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ENTITLED Modification of the MOSCED Equation to

Improve Predictions of Vapor-Liquid Equilibria

IS APPROVED BY ME AS FULFILLING THIS PART OF THE REQUIREMENTS FOR THE

DEGREE OF Bachelor of Sciences

Chemical Engineering

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**Modification of the ROSCED Equation
to Improve Predictions of Vapor-Liquid
Equilibria**

By

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Thesis

**for the
Degree of Bachelor of Science
in
Chemical Engineering**

**College of Liberal Arts and Sciences
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Summary

The project undertaken as a Chemical Engineering 292/390 assignment was to reparameterize the MOSCED equation. This equation predicts activity coefficients at infinite dilution which can be used to predict VLE behavior. Typically VLE behavior is predicted from the differences in two compounds of the energy required to remove a molecule from its environment due to physical and chemical interactions (its cohesive energy density). The MOSCED equation extends the applicability of such equations to polar and associating systems by assuming the cohesive energy density can be separated into independent, additive components.

The goal of this project was to redefine the equations relating these components to physically measurable quantities and to see if this change would improve the predictive ability of the equation. In order to reduce the number of adjustable parameters being used, the relations for α (acidity) and β (basicity) were redefined in terms of Kamlet-Taft α and β , which are properties of the compounds. Once the new α and β were defined, the rest of the parameters in the MOSCED equation needed to be refit to the experimental data. In order to expedite the process, this was done in a stepwise fashion so that only a limited number of parameters were allowed to vary at one time.

The initial data set utilized contained only alkane-alkane (solute-solvent) pairs. By doing this, only two terms, λ and d_{12} were being optimized. The results for this step were exceptionally good. When the predicted γ^{∞} 's were compared to the measured values, an average error of only 4.2% resulted with a maximum error of 18.1%. Further reparameterization was

attempted, but the progress was slowed by difficulties with the computer program (errors while running) and no sufficient results were obtained. It is evident that good predictions were accomplished for the alkane-alkane pairs. In fact the accuracy of these predictions is surprising since the data they were measured against is only considered to be accurate to 10%. It is recommended, based on these results, that the reparameterization continue until an adequate error is obtained.

Introduction

The project undertaken as a thesis assignment was to modify an existing equation representing vapor-liquid equilibrium (VLE) behavior. The equation studied, the MOSCED equation (70), was developed at this university by E. R. Thomas and C. A. Eckert.

The MOSCED equation (Modified Separation of Cohesive Energy Density) is an extension of the regular solution theory of VLE behavior (Scatchard, 1931 ; Hildebrand & Wood, 1933) to polar and associating systems. The cohesive energy density of a compound is the energy necessary to remove a molecule from its environment due to physical and chemical interactions with surrounding molecules. The MOSCED equation, following the lead of other investigators (Arkel & Vlex, 1936; Arkel, 1946; Blanks & Prausnitz, 1964; Welmer & Prausnitz, 1965; Gordon, 1966; Hansen, 1967; Helpinstill & VanWinkle, 1968; Nelson, et al., 1970; Keller, et al., 1971; Hsieh, 1973; Barton, 1975; Koenhen & Smolders, 1975; Karger, et al., 1976; Tijssen, et al., 1976; Karger & Snyder, 1978), separates the cohesive energy density terms into independent, additive components. Each component represents a certain physical or chemical property of the molecule. Thus the equation in its present form is :

$$\ln \gamma_2^\infty = v_2 / RT [(\lambda_1 - \lambda_2)^2 + q_1^2 q_2^2 (\tau_1 - \tau_2)^2 / \psi_1 + (\alpha_1 - \alpha_2)(\beta_1 - \beta_2) / \xi_1] + d_{12}$$

where 1 = solvent
 2 = solute
 γ^{∞} = activity coefficient at infinite dilution
 v = partial molar volume
 λ = polarizability
 q = dipole-induced dipole energy
 τ = polarity
 α = acidity
 β = basicity
 ϕ, ξ = asymmetry parameters
 d_{12} = combinatorial term to account for
differing molecular sizes

By predicting γ^{∞} , the vapor-liquid equilibrium can be characterized through relations such as the Wilson equation (71).

The equation in its present form has two main deficiencies. Firstly, each of the parameters in the equation is determined by an empirical relation composed of physically measurable properties of the compound and constants (1). Presently three of these relations (τ, α, β) contain adjustable parameters. The drawback associated with this is that if one uses enough adjustable parameters, any set of data can be fit with an equation. Although three adjustable parameters is not unreasonable for such an equation, reducing this number would increase the significance of the results.

The second deficiency has to do with the combinatorial term, d_{12} . When the mixture consists of small solute molecules in a solvent of large molecules the combinatorial term tends to be too large and thus overestimates γ^{∞} .

Objective

The objective of this research project was to address the first deficiency mentioned above. This was to be done by relating the α and β terms to Kamlet-Taft α and β 's (pp. A6-A19) which are physical attributes of the molecules. This reduced the number of adjustable parameters to one (τ). At the same time this was being done, the coefficients in the other empirical relations would be redefined to fit the data in light of the new α and β .

Strategy

Since ultimately 15 coefficients would have to be modified, it was necessary to devise a method to separate the coefficients into groups so that all of the coefficients would not be changing at one time. This greatly expedited the reparameterization process. The first step was to select a subset of data which would not require use of all the parameters. By using alkane-alkane (solute-solvent) pairs, only two interaction terms were involved - the dispersion term, λ , and the term to account for differences in molecular size, d_{12} . All of the other parameters for alkanes are zero, so the corresponding coefficients did not need to be optimized. This provided initial estimates of the optimum coefficients for λ and d_{12} .

The next step was to gradually increase the number of γ^{∞} data to which the equation was being fit. As the number of data increased, more parameters became involved. For this reason the coefficients for λ and d_{12} were left at their initial estimates (described above) while the other parameters were being optimized. This process would continue, increasing and decreasing the size of the data sets and iterating to final values of the optimum parameters.

Procedure

The majority of the work for this project was constructing the databases and computer programs in preparation for the coefficient optimization. The first database which was compiled was one containing Kamlet-Taft parameters. In addition to the α and β terms mentioned above, Kamlet-Taft parameters also include terms designated as π , α_m , β_m , and π_m . The π_m term is a measure of the polarizability of the compound. It may be incorporated into the MOSCED equation when the equation is restructured. The other terms are "monomer" terms which apply in very dilute solutions of the solute. The database was constructed on a Lotus 123 spreadsheet and includes 655 compounds (pp. A6-A19). All of the parameters in the database come from literature sources.

The next set of data that had to be compiled was one containing measured values of γ^{∞} 's. The starting point for this database was the data compiled by Wen Te Chen when completing his graduate work at this university. This data was imported to a Lotus file and edited. All records which did not have a literature reference were deleted. This resulted in a database very similar to the one utilized by E. R. Thomas in developing the original MOSCED equation.

Three data sets of γ^{∞} values were considered for use in the reparameterization process. The first was described above. The second was a subset of this database which represented data that had not been extrapolated. The third database consisted of a subset of the second database containing only those values which had been measured at 293-298^o K. For reasons described in the Appendix (pp. A106-A109), it was decided to use each of the latter two data sets in the reparameterization.

The next step was the actual reparameterization process. Initially this process was attempted using a program (GRG) on the university's CYBER network. This approach was abandoned rather quickly since a subroutine was available on a PC which would eliminate the time spent waiting to use the CYBER. The program constructed on the PC was designed to use a subroutine in the International Math and Statistics Library (IMSL) which performed a non-linear least squares fit to the data (subroutine ZXSSQ). Two obstacles were encountered with this subroutine. For some reason the program would not accept a γ database of more than 99 records. The source of this error was never found. The major drawback to this routine, however, was the fact that no constraints could be placed on the variables being optimized.

A suitable optimization subroutine was finally located on the school's VAX computer. This was another IMSL routine (ZXMWD) which did allow constraints on the variables. The subroutine and the program used are documented in the Appendix (pp. A110-A124).

Results

The initial results of this project proved to be very encouraging. When only the λ and d_{12} terms were fit to the alkane-alkane data, the 231 datapoints could be fit to within an average error of 4.2% and a maximum error of 18.1%. The parameters found are presented below and are compared with those from the original MOSCED equation.

original parameters : aa = 0.953

$$\lambda = 19.5 \left[\frac{(\eta_D^2 - 1)}{(\eta_D^2 + 2)} \right]$$

(aromatics)

$$\lambda = 20.3 \left[\frac{(\eta_D^2 - 1)}{(\eta_D^2 + 2)} \right]$$

(non-aromatics)

new parameters : aa = 0.859

$$\lambda = 18.859 \left[\frac{(\eta_D^2 - 1)}{(\eta_D^2 + 2)} \right]$$

Steps were taken toward reparameterizing more of the relations, but no conclusive results had been obtained at the time of this report.

Conclusions

From these results the following can be concluded:

1. The reparameterized MOSCED equation holds great potential in the realm of alkane-alkane γ prediction.
2. Further iterations are needed to determine the optimum coefficients for the MOSCED equation.

Based on the results of this project, it is recommended that the reparameterization continue until all of the parameters are optimized.

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Literature Cited

1. Thomas, E. R., Newman, B. A., Nicolaides, G. L., Eckert, C. A., J. Chem. Eng. Data, submitted 1981.
2. Thomas, E. R., Newman, B. A., Long, T. C., Wood, D. A., Eckert, C. A., Ibid, submitted 1981.
3. Gmehling, J., Onken, U., "Vapor-Liquid Equilibrium Data Collection", DECHEMA, 1977.
4. Rohrschneider, L., Anal. Chem., 45, 1241 (1973).
5. Zawidzki, J., Z. Phys. Chem., 35, 129 (1900).
6. Wilson, G. M., AIChE Symposium Series, 140 (70), 120 (1974).
7. Ino, M., J. Sudo, Hirata, M., J. Chem. Eng. Data, 15, 446 (1970).
8. Schreiber, L. B., Eckert, C. A., I. & E. C. Process Design & Devel., 10, 572 (1971).
9. Abraham, M. H., Grellier, P. L., Mana, J., J. Chem. Thermodynamics, 6, 1175 (1974).
10. Byer, S. M., Gibbs, R. E., van Ness, H. C., AIChE J., 19, 245 (1973).
11. Deal, C. H., Derr, E. L., Ind. Eng. Chem., Process Des. Dev., 3, 394 (1964).
12. Muthu, O., Maher, P. H., Smith, B. O., J. Chem. Eng. Data, 25, 163 (1980).
13. Gerster, J. A., John, A., Gorton, E. J., J. Chem. Eng. Data, 5, 423 (1960).
14. Locke, David C., Advances Chromatogn., 8, 47 (1969).
15. Maier, P. J., Smith, B. D., J. Chem. Eng. Data, 25, 61-68 (1980).
16. Sugi, H., Katayama, T., J. Chem. Eng. Japan, 11, 168 (1978).
17. Barker, P. E., Hilmi, A. K., J. Gas Chromatography, 5, 119 (1967).
18. Udovenko, V. V., Frid, T. B., Zh. Fiz. Khim., 22, 1263 (1948).
19. Pierotti, G. J., Deal, C. H., Derr, E. L., Ind. Eng. Chem. Fund., 51 95 (1959), and references cited therein.

20. Free, K. W., Hutchinson, H. P., J. Chem. Eng. Data, 4, 193 (1959).
21. Tochigi, K., Kojima, K., J. Chem. Eng. Japan, 9(4), 267 (1976).
22. Kikic, I., Alessi, P., Gozzi, P., Lapsin, R. L., Santis, R. O.,
Ibid., 25, 33 (1980).
23. Nagata, I., J. Chem. Eng. Japan, 276 (1976).
24. Chao, K. C., Ph.D. Thesis, University of Wisconsin, Madison, WI., 1956.
25. Sassa, Y., Katayana, T., J. Chem. Eng. Japan, 7, 1 (1974).
26. Funk, E. W., Pravenitz, J. M., Ind. Eng. Chem., 62, 8 (1970).
27. Ain, K., Fluid Phase Equilibria, 2, 119 (1978).
28. Nagata, I., Hayashida, H., J. Chem. Eng. Japan, 3, 161 (1970).
29. Brown, I., Smith, F., Austr. J. Chem., 12, 407 (1959).
30. Hosselini, S. M., Schneider, G., Z. Phys. Chem. (Frankfurt), 36
137 (1963).
31. Brzostowski, W., Warycha, S., Bull. Acad. Polon. Sci. Ser. Sci. Chem.
11, 539 (1963).
32. Monfort, J. P., Vidal, J., Renon, H., J. Chim. Phys., 67, 748 (1970).
33. Suryanarayana, Y. S., van Winkle, M., J. Chem. Eng. Data, 11, 7 (1966).
34. Tassios, D., van Winkle, M., Ibid., 12, 555 (1967).
35. Meyers, H. S., Petrol. Refiner, 36, 175 (1957).
36. Vernier, P., Raimbault, C., Renon, H., J. Chim. Phys., 66(1), 429
(1969).
37. Lerot, J.-C., Masson, J.-C., Renon, H., Fabrics, J.-F., Sannier, H.,
Ind. Eng. Chem., Process Des., Dev., 16(1), 139 (1977).
38. Pul'tsin, M. N., Galle, A. A., Proskuryakov, V. A., Russian Journal
of Phys. Chem., 47, 428 (1973).
39. Spelyng, W. A., Tassios, D. P., Ind. Eng. Chem. Process Des. Develop.,
13, 328 (1974).

40. Copp, J. L., Everett, D. H., Disc. Faraday Soc., 15, 174 (1960).
41. Nakanishi, K., Shirai, H., Minahiyama, T., Ibid., 12, 591 (1967).
42. Long, T. C., Ph.D. Thesis, University of Illinois, Urbana, Il., 1980.
43. Kojima, K., Tochigi, K., Ochi, K., Kagaku Kogaku, 38, 135 (1974).
44. Schneider, G., Z. Phys. Chem., 27, 171 (1961).
45. Lu, B. C. Y., Can. J. Technol., 34, 468 (1957).
46. Desty, D. H., Swanton, W. T., J. Phys. Chem., 65, 766 (1961).
47. Maher, P. J., Smith, B. D., Ibid., 24, 16 (1979).
48. Nitta, T., Katayama, T., J. Chem. Eng. Japan, 6, 224 (1973).
49. Aristovich, V. Y., Morachevskii, A. G., Sabylen, I. I., Zh. Prikl. Khim., 42, 1354 (1969).
50. Nagata, I., J. Chem. Eng. Data, 1, 367 (1962).
51. Scatchard, G., Raymond, C. I., J. Am. Chem. Soc., 60, 1278 (1938).
52. Kudryautseva, L. S., Susarev, M. P., Zh. Prikl. Khim., 36, 1231 (1963).
53. Scatchard, G., Wood, S. E., Mochel, J. M., J. Am. Chem. Soc., 68, 1960 (1946).
54. Nagata, I., J. Chem. Eng. Data, 14, 418 (1969).
55. Prabhu, P. S., van Winkle, M., J. Chem. Eng. Data, 8, 210 (1963).
56. Aristovich, V. Yu, Morachevskii, Sabylen, I. I., Zh. Prikl. Khim., 38, 2694 (1965).
57. Smiley, H., J. Chem. Eng. Data, 15(3), 413 (1970).
58. Kwantes, A., Rijnder, G. W. A., Gas Chromatography, Butterworth, London (1958), and references cited therein.
59. Littlewood, A. B., Anal. Chem., 36, 1441 (1964).
60. Richon, D., Antoine, P., Renon, H., Ind. Eng. Chem. Process Des. Dev., 19, 144 (1980).

61. Snyder, P. S., Thomas J. F., J. Chem. Eng. Data, 13, 527 (1968).
62. Comanita, V. J., Greenkorn, R. A., Chao, K., J. Chem. Eng. Data, 21(4), 491 (1976).
63. Harris, H. G., Prausnitz, J. M., J. Chromat. Sci., 7, 685 (1969).
64. Martire, D. E., Pollara, L. Z., J. Chem. Eng. Data, 10, 40 (1965).
65. Cruickshank, A. J. B., Gainey, B. W., Young, C. L., Trans. Faraday Soc., 64, 337 (1968).
66. Orgorodnikov, S. K., Kogan, V. B., Nentsov, M. S., Zh. Prikl. Khim., 34, 123 (1961).
67. Hanson, D. A., van Winkle, M., J. Chem. Eng. Data, 12, 319 (1967).
68. Myers, H. S., Ind. Eng. Chem., 48, 1104 (1956).
69. Parcher, J. F., Weiner, P. H., Hussey, C. I., Westlake, T. N., J. Chem. Eng. Data, 20(2), 145 (1975).

References

- 70 Thomas, E. R. and C. A. Eckert. Prediction of Limiting Activity Coefficients by a Modified Separation of Cohesive Energy Density Model and UNIFAC. I&EC Process Design and Development, 1984, 23, 194.
- 71 Wilson, G. M. Journal American Chem. Society, 86, 127 (1964).
- 72 Kamlet, M. J. , P. W. Carr, R. W. Taft, and M. H. Abraham. Linear Solvation Energy Relationships. J. Am. Chem. Soc., 103, 6062, 1981.
- 73 Taft, R. W., J. L. M. Abboud, and M. J. Kamlet. Linear Solvation Energy Relationships. J. Am. Chem. Soc., 103, 1080, 1981.
- 74 Kamlet, M. J. , J. L. M. Abboud, M. H. Abraham, and R. W. Taft. Linear Solvation Energy Relationships. J. Org. Chem. Soc., 48, 2877, 1983.
- 75 Taft, R. W., J. L. M. Abboud, M. J. Kamlet, and M. H. Abraham. Linear Solvation Energy Relationships. J. Soln. Chem., 14, 153, 1985.

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Appendix

Nomenclature

SLT	=	solute
SLV	=	solvent
ID	=	identification #
INUM	=	# of skeletal carbon atoms
RI = n_D	=	refractive index
γ^∞	=	infinite dilution activity coefficient
T	=	temperature ($^\circ$ K)
GAMCLC	=	calculated γ^∞
REF	=	literature reference
IER	=	IMSL error code
IMSL	=	International Math & Statistics Libraries

-A3-
MOSCED PARAMETERS

ID	RI	V	Q	IGRP	IGTP	INUM
1	1.628	72.0	1.00	10	001	001
2	1.460	96.5	1.00	02	001	001
3	1.506	98.5	1.00	02	001	001
4	1.446	80.7	1.00	02	001	001
5	1.496	82.7	1.00	02	001	001
6	1.424	64.1	1.00	02	001	001
7	1.542	69.6	1.00	02	001	001
8	1.328	40.5	1.00	03	001	001
9	1.381	53.7	1.00	07	001	001
10	1.531	79.1	1.00	02	001	001
11	1.344	52.2	1.00	05	002	002
12	1.438	99.6	1.00	02	002	002
13	1.471	92.7	1.00	02	002	002
14	1.445	79.1	1.00	02	002	002
15	1.416	84.2	1.00	02	002	002
16	1.392	72.0	1.00	07	002	002
17	1.513	93.6	1.00	02	002	002
18	1.424	76.5	1.00	02	002	002
19	1.361	58.4	1.00	03	002	002
20	1.366	70.4	1.00	05	003	003
21	1.359	74.4	1.00	04	003	003
22	1.360	80.4	1.00	06	002	003
23	1.361	79.3	1.00	06	002	003
24	1.402	89.0	1.00	07	003	003
25	1.430	77.0	1.00	10	001	003
26	1.394	90.1	1.00	07	003	003
27	1.503	111.6	1.00	02	003	003
28	1.388	88.1	1.00	02	003	003
29	1.434	90.9	1.00	02	003	003
30	1.290	88.1	1.00	00	003	003
31	1.386	74.8	1.00	03	003	003
32	1.379	89.6	1.00	04	004	004
33	1.378	96.3	1.00	06	003	004
34	1.407	81.1	1.00	06	004	004
35	1.377	97.3	1.00	06	003	004
36	1.372	97.8	1.00	06	002	004
37	1.422	84.2	1.00	10	002	004
38	1.397	106.0	1.00	02	004	004
39	1.402	104.5	1.00	02	004	004
40	1.386	109.9	1.00	02	004	004
41	1.440	107.4	1.00	02	004	004
42	1.333	100.4	1.00	00	004	004
43	1.399	91.5	1.00	03	004	004
44	1.510	80.5	0.90	09	105	005
45	1.430	100.8	0.80	01	005	005
46	1.422	100.0	0.80	01	004	005
47	1.407	94.1	1.00	00	205	005

ID	RI	V	Q	IGRP	IGTP	INUM
48	1.387	105.9	0.90	01	005	005
49	1.383	107.0	0.90	01	005	005
50	1.371	109.6	0.90	01	005	005
51	1.338	107.8	1.00	01	004	005
52	1.364	111.8	0.90	01	004	005
53	1.388	107.3	1.00	04	004	005
54	1.453	90.9	1.00	03	205	005
55	1.392	105.8	1.00	04	005	005
56	1.390	106.5	1.00	04	005	005
57	1.384	115.0	1.00	06	003	005
58	1.388	113.7	1.00	06	004	005
59	1.384	114.5	1.00	06	003	005
60	1.445	124.0	1.00	02	005	005
61	1.358	115.3	1.00	00	005	005
62	1.354	116.4	1.00	00	004	005
63	1.410	108.1	1.00	03	005	005
64	1.552	102.3	0.90	08	106	006
65	1.525	101.8	0.90	08	106	006
66	1.501	89.1	0.90	08	106	006
67	1.551	89.0	0.90	03	106	006
68	1.586	91.1	0.90	08	106	006
69	1.447	101.4	0.92	01	206	006
70	1.451	103.6	1.00	04	206	006
71	1.392	123.8	0.92	01	005	006
72	1.426	108.1	1.00	00	206	006
73	1.388	125.0	0.92	01	006	006
74	1.383	126.7	0.92	01	005	006
75	1.410	112.4	1.00	00	206	006
76	1.400	122.6	0.92	01	005	006
77	1.396	125.1	1.00	04	005	006
78	1.467	105.4	1.00	03	206	006
79	1.392	132.0	1.00	06	004	006
80	1.375	130.8	1.00	00	006	006
81	1.375	130.3	1.00	00	004	006
82	1.377	129.7	1.00	00	005	006
83	1.369	132.9	1.00	00	004	006
84	1.382	149.0	1.00	00	005	007
85	1.372	131.9	1.00	00	005	007
86	1.418	124.7	1.00	03	006	007
87	1.401	139.0	1.00	09	002	007
88	1.528	102.6	0.90	08	106	007
89	1.539	117.2	0.90	08	106	007
90	1.564	128.4	0.90	08	106	007
91	1.497	106.3	0.90	08	106	007
92	1.517	109.1	0.90	08	106	007
93	1.420	137.2	1.00	05	008	007
94	1.423	124.4	1.00	00	207	007
95	1.400	140.9	0.93	01	007	007
96	1.444	121.3	1.00	00	207	007

ID	RI	V	Q	IGRP	IGTP	INUM
97	1.406	139.5	1.00	04	007	007
98	1.388	146.6	1.00	00	007	007
99	1.389	145.8	1.00	00	006	007
100	1.392	148.7	1.00	00	005	007
101	1.534	116.9	0.90	08	106	008
102	1.496	122.5	0.90	08	106	008
103	1.496	123.3	0.90	08	106	008
104	1.506	120.6	0.90	08	106	008
105	1.459	134.4	1.00	00	008	008
106	1.409	157.0	0.94	01	008	008
107	1.433	142.4	1.00	00	008	008
108	1.391	165.1	1.00	00	007	008
109	1.397	162.6	1.00	00	008	008
110	1.430	157.8	1.00	03	008	008
111	1.627	118.1	0.90	08	106	009
112	1.527	132.9	0.90	08	106	009
113	1.523	142.4	0.90	08	106	009
114	1.427	163.8	1.00	00	007	009
115	1.420	173.1	1.00	04	009	009
116	1.412	176.6	1.00	04	007	009
117	1.405	178.7	1.00	00	009	009
118	1.418	189.6	1.00	09	003	009
119	1.658	139.6	0.90	08	110	010
120	1.490	156.0	0.90	08	106	010
121	1.481	154.0	0.90	00	210	010
122	1.430	186.9	1.00	05	011	010
123	1.441	175.5	1.00	00	010	010
124	1.421	189.3	0.95	01	010	010
125	1.506	143.6	1.00	06	008	010
126	1.412	194.9	1.00	00	010	010
127	1.437	190.8	1.00	03	010	010
128	1.422	227.5	1.00	00	012	012
129	1.445	286.0	1.00	09	016	015
130	1.441	287.3	0.97	01	016	016
131	1.451	301.5	1.00	02	016	016
132	1.462	305.6	1.00	02	016	016
133	1.435	292.8	1.00	00	016	016
134	1.449	288.0	1.00	03	016	016
135	1.439	327.1	1.00	00	018	018
136	1.443	358.3	1.00	00	020	020
137	1.444	374.6	1.00	00	021	021
138	1.448	423.8	1.00	00	024	024
139	1.452	489.4	1.00	00	028	028
140	1.499	478.5	0.87	01	034	030
141	1.454	522.2	1.00	00	030	030
142	1.453	522.0	1.00	00	034	030
143	1.455	555.0	1.00	00	032	032
144	1.457	604.4	1.00	00	035	035

ID	PI STAR	ALPHA	BETA	PI m	ALPHA m	BETA m
48						
49						
50	0.08		0.07		0.00	
51						
52						
53			0.48			
54						
55	0.72		0.45			
56	0.65		0.48		0.03	
57	0.53		0.45		0.00	
58	0.53		0.45		0.00	
59	0.53	0.00	0.45		0.00	
60						
61	-0.08	0.00	0.00		0.00	
62						
63	0.40		0.45		0.33	
64	1.01	0.00	0.30		0.00	
65	0.71	0.00	0.07		0.00	
66	0.59	0.00	0.10		0.00	
67	0.72		0.33		0.61	
68	0.73		0.50a		0.16	
69	0.10		0.10		0.00	
70	0.76		0.53		0.00	
71						
72	0.00	0.00	0.00		0.00	
73	0.08		0.07		0.00	
74						
75						
76						
77						
78	0.45		0.51		0.31	
79	0.51		0.45		0.00	
80	-0.04	0.00	0.00		0.00	
81						
82						
83						
84						
85	-0.02		0.00		0.00	
86	0.40		0.45		0.33	
87	0.14	0.00	0.71		0.00	
88	0.90	0.00	0.37		0.00	
89						
90						
91	0.55	0.00	0.11		0.00	
92	0.73	0.00	0.32a		0.00	
93						
94						
95						
96	0.05		0.00		0.00	

-A6-
KAMLET-TAFT PARAMETERS

ID	PI STAR	ALPHA	BETA	PI m	ALPHA m	BETA m
1	0.00	0.00	0.00	0.00	0.00	0.00
2	0.28		0.10		0.00	0.00
3					0.00	
4	0.58	0.44	0.10		(0.35)c	
5						
6	0.82	0.30	0.05			
7						
8	0.40	0.93	0.42	0.39	0.35	0.41
9	0.85	0.22	0.25		(0.19)c	
10		0.00	0.00			
11	0.75	0.19	0.31		(0.15)c	
12	0.49	0.00	0.10		0.00	
13						
14	0.81	0.00	0.10		0.00	
15						
16	0.80		0.25		0.00	
17						
18		0.00				
19	0.40	0.83	0.45	0.39	0.33	0.47
20	0.70		0.31		0.00	
21	0.71	0.08	0.48		0.04	
22	0.61	0.00	0.36		0.00	
23	0.60	0.00	0.42		0.00	
24	0.78		0.25		0.00	
25	0.88	0.00	0.69		0.00	
26	0.75		0.27		0.00	
27						
28						
29						
30						
31	0.40	0.78	0.45		0.33	
32	0.67	0.06	0.48		0.03	
33	0.55		0.45		0.00	
34	0.58	0.00	0.55		0.00	
35	0.60		0.38		0.00	
36	0.55	0.00	0.45		0.00	
37	0.55	0.00	0.37			
38						
39	0.39	0.00	0.00			
40						
41						
42	-0.11		0.00		0.00	
43	0.40	0.79	0.45		0.33	
44	0.87	0.00	0.64		0.00	
45						
46						
47	-0.01	0.00	0.00		0.00	

ID	PI STAR	ALPHA	BETA	PI m	ALPHA m	BETA m
97						
98	-0.02	0.00	0.00		0.00	
99						
100						
101	0.90		0.49		0.03	
102	0.53		0.12		0.00	
103	0.51	0.00	0.12		0.00	
104	0.51		0.12		0.00	
105	0.11	0.00	0.00		0.00	
106						
107						
108	-0.04	0.00	0.00			
109	0.01	0.00	0.00		0.00	
110	0.40		0.45		0.33	
111	0.92	0.00	0.64		0.00	
112	0.88		0.49		0.00	
113	1.19b		0.52a		0.00	
114						
115						
116						
117	0.02	0.00	0.00		0.00	
118						
119						
120	0.49		0.12		0.00	
121						
122						
123						
124						
125						
126	0.03		0.00		0.00	
127						
128	0.05	0.00	0.00		0.00	
129						
130						
131						
132						
133	0.08	0.00	0.00		0.00	
134						
135						
136						
137						
138						
139						
140						
141						
142	0.12					
143						
144						
145	0.04	0.00	0.00		0.00	

ID	PI STAR	ALPHA	BETA	PI m	ALPHA m	BETA m
146	0.06	0.00	0.00		0.00	
147	0.07	0.00	0.00		0.00	
148	0.07	0.00	0.00		0.00	
149	-0.06		0.00		0.00	
150	0.00		0.00		0.00	
151	-0.04		0.00		0.00	
152			0.00		0.00	
153	0.08		0.07		0.00	
154	0.10		0.11		0.00	
155	0.20		0.16			
156	0.20		0.14		d	
157	0.20		0.19		d	
158	0.47		0.10		d	
159	0.39		0.10		0.00	
160	0.37		0.10		0.00	
161	0.35		0.10		0.00	
162	0.33		0.10		0.00	
163	0.31		0.10		0.00	
164	0.82	0.30	0.10		(0.25)c	
165	0.95		0.10		d	
166	0.62		0.10		d	
167	0.44	0.00	0.05		0.00	
168	0.53	0.00	0.05		0.00	
169	0.28	0.00	0.05		0.00	
170	0.75	0.00	0.05		0.00	
171	0.22		0.10		0.00	
172	0.51	0.00	0.12		0.00	
173	0.47		0.13		0.00	
174	0.47		0.13		0.00	
175	0.47		0.13		0.00	
176	0.43		0.15		0.00	
177	0.43		0.15		0.00	
178	0.43		0.15		0.00	
179	0.39		0.17		0.00	
180	0.35		0.19		0.00	
181	0.51		0.12		0.00	
182	0.51		0.12		0.00	
183	0.49		0.12		0.00	
184	0.47		0.13		0.00	
185	0.47		0.12		0.00	
186	0.62	0.00	0.07		0.00	
187	0.79	0.00	0.06		0.00	
188	0.81	0.00	0.05		0.00	
189	0.80	0.00	0.03		0.00	
190	0.75	0.00	0.03		0.00	
191	0.70		0.03		0.00	
192	0.85		0.00		0.00	
193	0.75		0.00		0.00	
194	0.70		0.00		0.00	

ID	PI STAR	ALPHA	BETA	PI m	ALPHA m	BETA m
195	0.80		0.00		0.00	
196	0.80		0.00		0.00	
197	0.70		0.00		0.00	
198	0.75		0.00		0.00	
199	0.70		0.00		0.00	
200	0.80		0.02		0.00	
201	0.79		0.02		0.00	
202	0.67		0.08		0.00	
203	0.67		0.08		0.00	
204	0.67		0.08		0.00	
205	0.27	0.00	0.47		0.00	
206	0.27	0.00	0.46		0.00	
207	0.24	0.00	0.46		0.00	
208	0.27	0.00	0.47		0.00	
209	0.51	0.00	0.54		0.00	
210	-0.35		0.30		0.00	
211	0.69		0.33a		0.00	
212	0.69		0.33a		0.00	
213	0.69		0.33a		0.00	
214	0.73		0.22		0.00	
215	0.69	0.00	0.30a		0.00	
216	0.67		0.30		0.00	
217	0.86b		0.56		0.00	
218	0.62	0.00	0.37		0.00	
219	0.49		0.45		0.00	
220	0.51		0.45		0.00	
221	0.51		0.45		0.00	
222	0.49		0.45		0.00	
223	0.49		0.45		0.00	
224	0.70	0.00	0.35		0.00	
225	0.61	0.00	0.25		0.00	
226	0.65		0.37		0.00	
227	0.63		0.38		0.00	
228	0.63		0.36		0.00	
229	0.76	0.00	0.39		0.00	
230	0.74	0.00	0.41		0.00	
231	0.71		0.40		0.00	
232	1.14b		0.55a		0.00	
233	1.12b		0.55a		0.00	
234	1.19b		0.52a		0.00	
235	1.12b		0.55a		0.00	
236	1.32b		0.50a		0.00	
237	1.14b		0.52a		0.00	
238	1.10b		0.53a		0.00	
239	1.10b		0.53a		0.00	
240	1.10b		0.53a		0.00	
241	1.24b		0.42		0.00	
242	1.19b		0.42		0.00	
243	1.14b		0.42		0.00	

-All-

ID	PI STAR	ALPHA	BETA	PI m	ALPHA m	BETA m
244	1.14b		0.47a		0.00	
245	1.24b		0.42		0.00	
246	1.21b		0.68a		0.00	
247	0.67		0.42		0.00	
248	0.65		0.41		0.00	
249	0.63		0.41		0.00	
250	0.61		0.41		0.00	
251	0.59		0.41		0.00	
252	0.92	0.00	0.44		0.00	
253	0.75		0.36		0.00	
254	0.63		0.48		0.03	
255	0.61		0.48		0.03	
256	0.76		0.52		0.00	
257	0.95		0.45		0.03	
258	0.90		0.45		0.03	
259	0.90		0.45		0.03	
260	0.90		0.47		0.03	
261	0.86		0.50		0.03	
262	1.30		0.58a		0.04	
263	1.22		0.58a		0.04	
264	0.32		0.70		0.00	
265	0.31		0.69		0.00	
266	0.31		0.69		0.00	
267	0.30		0.69		0.00	
268	0.30		0.69		0.00	
269	0.29		0.69		0.00	
270	0.29		0.69		0.00	
271	0.25		0.70		0.00	
272	0.25		0.70		0.00	
273	0.25		0.70		0.00	
274	0.16		0.65		0.00	
275	0.14	0.00	0.69		0.00	
276	0.69		0.51a		0.13	
277	0.69		0.51a		0.13	
278	0.69		0.51a		0.13	
279	0.78		0.40a		0.20	
280	0.73		0.40a		0.20	
281	0.84		0.40a		0.20	
282	0.79		0.40		0.20	
283	0.78		0.45		0.18	
284	0.73		0.45		0.18	
285	(1.15)c		0.46		0.39	
286	(1.25)c		0.48		0.47	
287	1.32b		0.60a		0.16	
288	1.46b		1.00a		0.32	
289	0.83		0.50a		0.16	
290	0.83		0.50a		0.16	
291	0.73		0.47a	(0.12)c		
292	0.74		0.47a	(0.12)c		

ID	PI STAR	ALPHA	BETA	PI m	ALPHA m	BETA m
293	0.75	0.00	0.43a		0.00	
294	0.69		0.44a		0.00	
295	0.75		0.44a		0.00	
296	0.75b		0.67a		0.00	
297	0.84	0.00	0.67		0.00	
298	0.92		0.53		0.00	
299	0.87		0.53		0.00	
300	0.92	0.00	0.51		0.00	
301	0.87		0.51		0.00	
302	0.68		0.31		0.00	
303	1.34b		0.41a		0.00	
304	1.29b		0.41a		0.00	
305	0.80		0.28		0.00	
306	0.76		0.25		0.00	
307	0.74		0.25		0.00	
308	0.97		0.31		0.00	
309	0.97		0.31		0.00	
310	1.11		0.26		0.00	
311	1.06		0.26		0.00	
312	1.01		0.26		0.00	
313	1.16		0.26		0.00	
314	1.16		0.26		0.00	
315	1.06		0.55		0.00	
316	1.01		0.55		0.00	
317	0.76		0.15		0.00	
318	0.88	0.00	0.76		0.00	
319	0.84		0.78		0.00	
320	0.94		0.75		0.49	
321	1.00	0.00	0.76		0.00	
322	(1.30)c		0.73		0.00	
323	0.36		0.25		0.00	
324	0.36	0.00	0.28		0.00	
325	(0.80)c		0.20		0.00	
326	0.35		0.13		(0.10)c	
327	0.35		0.22		(0.10)c	
328	0.35		0.16		(0.10)c	
329	0.40		0.45		0.33	
330	0.40		0.45		0.33	
331	0.40		0.45		0.33	
332	0.40		0.45		0.33	
333	0.40		0.45		0.33	
334	0.40		0.45		0.33	
335	0.40		0.45		0.33	
336	0.40		0.45		0.33	
337	0.40		0.45		0.33	
338	0.45		0.43		0.33	
339	0.45		0.48		0.33	
340	0.40	0.76	0.51		0.31	
341	0.40		0.51		0.31	

ID	PI STAR	ALPHA	BETA	PI m	ALPHA m	BETA m'
342	0.40		0.51		0.31	
343	0.40		0.51		0.31	
344	0.40		0.51		0.31	
345	0.40		0.51		0.31	
346	0.40		0.51		0.31	
347	0.40		0.51		0.31	
348	0.40		0.51		0.31	
349	0.40		0.51		0.31	
350	0.40		0.51		0.31	
351	0.40		0.51		0.31	
352	0.40		0.51		0.31	
353	0.40		0.51		0.31	
354	0.45		0.53		0.33	
355	0.45		0.52		0.33	
356	0.45		0.52		0.33	
357	0.40	0.68	0.57	0.39	0.29	0.56
358	0.40		0.57		0.29	
359	0.40		0.57		0.29	
360	0.40		0.57		0.29	
361	0.40		0.57		0.29	
362	0.40		0.57		0.29	
363	0.40		0.57		0.29	
364	0.40		0.57		0.29	
365	0.99b		0.52a		0.35	
366	0.95b		0.53a		0.35	
367	0.95b		0.53a		0.35	
368	1.11b		0.42		0.36	
369	1.11b		0.42		0.36	
370	0.97		0.55		0.33	
371	0.95		0.55		0.33	
372	0.99		0.61		0.29	
373	1.04		0.55		0.35	
374	0.68		0.34		0.58	
375	0.68		0.34		0.58	
376	0.77		0.23		0.69	
377	0.72		0.23		0.69	
378	0.84		0.23		0.69	
379	0.79		0.23		0.69	
380	0.78		0.28		0.65	
381	0.73		0.28		0.65	
382	0.82		0.33		0.61	
383	0.92		0.33		0.61	
384	0.65		0.38		1.05	
385	0.60	1.12	0.45	0.41	0.71	
386	0.58		0.45		0.67	
387	0.56		0.45		0.60	
388	0.54		0.45		0.56	
389	0.52		0.45		0.55	
390	0.42		0.45		0.55	

ID	PI STAR	ALPHA	BETA	PI m	ALPHA m	BETA m
391	0.74		0.40		0.75	
392	0.70		0.41		0.73	
393	0.70		0.41		0.73	
394	0.79		0.36		0.79	
395	0.74		0.36		0.79	
396	0.84		0.36		0.79	
397	0.79		0.36		0.79	
398	0.79		0.38		0.77	
399	0.74		0.38		0.77	
400	1.19b		0.55a		0.65	
401	1.15b		0.56a		0.64	
402	1.31b		0.45		0.67	
403	1.31b		0.45		0.67	
404	1.39b		0.45		0.67	
405	1.22b		0.50a		0.66	
406	1.22b		0.50a		0.66	
407	1.22b		0.50a		0.66	
408	1.17b		0.55a		0.65	
409	1.15b		0.55a		0.65	
410	0.84		0.40		0.55	
411	0.70		0.15		0.00	
412	0.66		0.16		0.00	
413	0.66		0.16		0.00	
414	0.62		0.17		0.00	
415	0.62		0.17		0.00	
416	0.62		0.17		0.00	
417	0.62		0.17		0.00	
418	0.62		0.17		0.00	
419	0.64		0.17		0.00	
420	0.20		0.18		0.00	
421	0.82		0.11		0.00	
422	0.82		0.11		0.00	
423	1.12		0.30		0.00	
424	0.80		0.20		0.00	
425	0.76		0.21		0.00	
426	0.76		0.21		0.00	
427	0.72		0.22		0.00	
428	0.80		0.20		0.00	
429	0.76		0.21		0.00	
430	0.91		0.16		0.00	
431	0.90		0.25		0.00	
432	0.86		0.26		0.00	
433	0.86		0.26		0.00	
434	0.86		0.26		0.00	
435	0.82		0.27		0.00	
436	0.84		0.27		0.00	
437	0.90		0.25		0.00	
438	0.90		0.25		0.00	
439	0.86		0.26		0.00	

ID	PI STAR	ALPHA	BETA	PI m	ALPHA m	BETA m
440	0.86		0.26		0.00	
441	0.82		0.27		0.00	
442	0.90		0.25		0.00	
443	1.00		0.30		0.00	
444	1.00		0.30		0.00	
445	0.90		0.25		0.00	
446	1.00		0.30		0.00	
447	1.00		0.30		0.00	
448	0.96		0.31		0.00	
449	1.00		0.30		0.00	
450	1.10		0.35		0.00	
451	0.66		0.21		0.00	
452	0.62		0.22		0.00	
453	0.76		0.26		0.00	
454	0.76		0.26		0.00	
455	0.62		0.17		0.00	
456	0.80		0.25		0.00	
457	0.90		0.30		0.00	
458	0.90		0.30		0.00	
459	0.90		0.30		0.00	
460	0.82		0.27		0.00	
461	0.78		0.28		0.00	
462	0.92		0.64		0.00	
463	0.88		0.65		0.00	
464	1.02		0.69		0.00	
465	1.02		0.64		0.00	
466	1.22		0.74		0.00	
467	1.84		1.28		0.00	
468	1.18b		0.20a		0.00	
469	1.20b		0.17a		0.00	
470	1.42b		0.14a		0.00	
471	1.29b		0.13a		0.00	
472	1.34b		0.17a		0.00	
473	1.46b		0.10a		0.00	
474	1.34b		0.10a		0.00	
475	1.29b		0.10a		0.00	
476	1.48b		0.07a		0.00	
477	1.39b		0.10a		0.00	
478	1.45b		0.03a		0.00	
479	1.34b		0.10a		0.00	
480	1.70b		0.00a		0.00	
481	1.50b		0.00a		0.00	
482	1.46b		0.07a		0.00	
483	1.40b		0.00a		0.00	
484	1.55b		0.00a		0.00	
485	1.40b		0.00a		0.00	
486	1.45b		0.00a		0.00	
487	1.50b		0.00a		0.00	
488	1.10b		0.22a		0.00	

IO	PI STAR	ALPHA	BETA	PI m	ALPHA m	BETA m
489	-0.41	0.00	0.00			
490	0.58	0.44	0.05			
491	0.71	0.08	0.48			
492	0.73	1.51	0.00		0.74	0.00
493	0.88	0.00	0.69			
494	0.97	0.71				
495	1.09	1.17	0.50	0.39	0.30	0.20
496	0.65	1.96	0.00		0.95	0.00
497			0.14			
498		0.00	0.44			
499			0.19			
500			0.25			
501			0.61			
502			0.77			
503			0.78			
504			0.79			
505			1.06			
506	0.76	0.00				
507	0.64	0.00				
508	0.41	0.00				
509	0.67	0.00				
510	0.61					
511	0.59					
512	0.66					
513	0.35					
514	0.35	0.00				
515	0.58	0.00				
516	-0.39	0.00	0.00			
517	-0.41	0.00	0.00			
518	0.41	0.00				
519	0.67					
520	0.65					
521	0.64					
522	0.63					
523	0.62					
524	0.56					
525	0.53	0.00	0.41			
526	0.66	0.00	0.13			
527	0.87	0.00	0.49			
528	0.46	0.00				
529	0.64					
530	0.83	0.00	0.40			
531	0.16	0.00	0.62			
532	0.98	0.00				
533	0.39	0.00	0.00			
534	0.07					
535	0.24					
536	0.35					
537	0.50					

ID	PI	STAR	ALPHA	BETA	PI m	ALPHA m	BETA m
538		0.58					
539		0.59					
540		0.64					
541			0.00	0.00			
542		0.92	0.90	0.52			
543		0.80	0.00	0.41			
544		0.63		0.53			
545		0.66		0.52			
546		0.83	0.00	0.80			
547		0.30					
548		0.69	0.00				
549		0.72	0.00	0.77			
550		0.84	0.00	0.67			
551		0.80	0.00	0.76			
552		0.92		0.00			
553		1.12		0.00			
554		0.41	0.68	1.01			
555		0.73	1.51	0.00			
556		0.65	1.96	0.00			
557		0.72					
558		0.71					
559		0.67		0.48			
560		0.88		0.76			
561		0.92	0.00	0.77			
562		0.87		1.05			
563				0.48			
564				0.79			
565				0.44			
566				0.31			
567				0.34			
568				0.54			
569				0.58			
570				0.66			
571			0.00	0.32			
572			0.00	0.42			
573			0.00	0.49			
574			0.00	0.59			
575			0.00	0.43			
576			0.00	0.48			
577			0.00	0.53			
578				0.42			
579				0.46			
580				0.51			
581	0.45		0.00	0.42			
582	0.39		0.00				
583			0.00	0.39			
584			0.00	0.40			
585			0.00	0.38			
586			0.00	0.19			

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ID	PI STAR	ALPHA	BETA	PI m	ALPHA m	BETA m
587		0.00	0.62			
588		0.00	0.61			
589		0.00	0.72			
590		0.00	0.77			
591		0.00	0.78			
592		0.00	0.70			
593		0.00	0.73			
594		0.00	0.64			
595		0.00	0.71			
596		0.00	0.78			
597		0.00	0.65			
598		0.00	0.75			
599		0.00	0.61			
600		0.00	0.16			
601		0.00	0.20			
602		0.00	0.20			
603		0.00	0.16			
604	0.16	0.00	0.62			
605	0.49	0.00	0.57			
606		0.00	0.54			
607		0.00	0.68			
608		0.00	0.71			
609			0.37			
610			0.57			
611			0.60			
612			0.63			
613		0.00	0.80			
614		0.00	0.82			
615		0.00	0.73			
616		0.00	0.70			
617		0.00	0.83			
618		0.00	0.71			
619		0.00	0.60			
620		0.00	0.45			
621		0.00	0.45			
622		0.00	0.46			
623		0.00	0.72			
624		0.00	0.78			
625		0.00	0.80			
626	0.87	0.00	1.05			
627	0.65	0.00				
628		0.00	0.94			
629		0.00				
630		0.00	1.02			
631		0.00	0.62			
632		0.00	0.68			
633		0.00	0.74			
634		0.00	0.79			
635		0.00	0.74			

ID	PI STAR	ALPHA	BETA	PI m	ALPHA m	BETA m
636		0.00	0.76			
637		0.00	0.80			
638		0.00	0.81			
639		0.00	0.84			
640		0.00	0.88			
641		0.00	1.04			
642		0.00	1.05			
643		0.00	0.46			
644		0.00	0.48			
645		0.00	0.53			
646		0.00	0.78			
647		0.00	0.42			
648		0.00	0.87			
649		0.00	0.66			
650		0.00	0.48			
651		0.00	0.74			
652		0.00	0.72			
653	0.80	0.00				
654	0.33	0.00	0.00			
655	0.36	0.00				

FOOTNOTES

- a) These are the sum of beta values for hydrogen bonding at multiple sites.
- b) These are the sum of pi star values for aliphatic and aromatic moieties or for two non-fused rings.
- c) These values are particularly uncertain.
- d) The parameters are intended to be used only in situations where there is only a minor dependence on alpha m ; in these circumstances use alpha m = 0.20 as a first approximation.
- e) These values are to be used only in aqueous solubility correlations. For correlations of solvent/water partition coefficients, subtract 0.20 from these values.

10 COMPOUND

- 1 CARBON DISULFIDE
- 2 CARBON TETRACHLORIDE
- 3 BROMOTRICHLOROMETHANE
- 4 CHLOROFORM
- 5 BROMODICHLOROMETHANE
- 6 DICHLOROMETHANE
- 7 DIBROMOMETHANE
- 8 METHANOL
- 9 NITROMETHANE
- 10 METHYL IODIDE
- 11 ACETONITRILE
- 12 1,1,1-TRICHLOROETHANE
- 13 1,1,2-TRICHLOROETHANE
- 14 1,2-DICHLOROETHANE
- 15 1,1-DICHLOROETHANE
- 16 NITROETHANE
- 17 ETHYL IODIDE
- 18 ETHYL BROMIDE
- 19 ETHANOL
- 20 PROPIONITRILE
- 21 ACETONE
- 22 ETHYL FORMATE
- 23 METHYL ACETATE
- 24 1-NITROPROPANE
- 25 DIMETHYL FORMAMIDE
- 26 2-NITROPROPANE
- 27 2-PROPYL IODIDE
- 28 N-PROPYL CHLORIDE
- 29 N-PROPYL BROMIDE
- 30 N-PROPANE
- 31 N-PROPANOL
- 32 2-BUTANONE
- 33 METHYL PROPIONATE
- 34 TETRAHYDROFURAN
- 35 N-PROPYL FORMATE
- 36 ETHYL ACETATE
- 37 DIOXANE
- 38 2-CHLOROBUTANE
- 39 N-BUTYL CHLORIDE
- 40 T-BUTYL CHLORIDE
- 41 N-BUTYL BROMIDE
- 42 N-BUTANE
- 43 N-BUTANOL
- 44 PYRIDINE
- 45 TRANS-1,3-PENTADIENE
- 46 ISOPRENE
- 47 CYCLOPENTANE
- 48 1-PENTENE

ID COMPOUND
49 2-PENTENE
50 1-PENTENE
51 2-METHYL BUTENE
52 3-METHYL BUTENE
53 METHYL ISOPROPYL KETONE
54 CYCLOPENTANOL
55 3-PENTANONE
56 2-PENTANONE
57 N-PROPYL ACETATE
58 METHYL BUTYRATE
59 ETHYL PROPIONATE
60 N-PENTYL BROMIDE
61 N-PENTANE
62 ISOPENTANE
63 1-PENTANOL
64 NITROBENZENE
65 CHLOROBENZENE
66 BENZENE
67 PHENOL
68 ANILINE
69 CYCLOHEXENE
70 CYCLOHEXANONE
71 4-METHYL PENTENE
72 CYCLOHEXANE
73 1-HEXENE
74 2-METHYL-1-PENTENE
75 METHYL CYCLOPENTANE
76 2-METHYL-2-PENTENE
77 4-METHYL-2-PENTANONE
78 CYCLOHEXANOL
79 N-BUTYL ACETATE
80 N-HEXANE
81 2,3-DIMETHYL BUTANE
82 3-METHYL PENTANE
83 2,2-DIMETHYL BUTANE
84 2,4-DIMETHYL PENTANE
85 2-METHYL PENTANE
86 N-HEXANOL
87 TRIETHYLAMINE
88 BENZONITRILE
89 BENZYL CHLORIDE
90 BROMOANISOLE
91 TOLUENE
92 ANISOLE
93 HEPTANENITRILE
94 METHYL CYCLOHEXANE
95 1-HEPTENE
96 CYCLOHEPTANE
97 ETHYL BUTYL KETONE

ID COMPOUND
98 N-HEPTANE
99 3-METHYL HEXANE
100 2,2-DIMETHYLPENTANE
101 ACETOPHENONE
102 ETHYL BENZENE
103 P-XYLENE
104 O-XYLENE
105 CYCLOOCTANE
106 1-OCTENE
107 ETHYL CYCLOHEXANE
108 ISOCTANE
109 N-OCTANE
110 N-OCTANOL
111 QUINOLINE
112 PROPIOPHENONE
113 BENZYL ACETATE
114 1,3,5-TRIMETHYLCYCLOHEXANE
115 DIBUTYL KETONE
116 DIISOBUTYL KETONE
117 N-NONANE
118 TRIPROPYLAMINE
119 BROMONAPHTHALENE
120 N-BUTYL BENZENE
121 DECALIN
122 DECANENITRILE
123 BUTYL CYCLOHEXANE
124 1-DECENE
125 ETHYL OCTANOATE
126 N-DECANE
127 N-DECANOL
128 N-DODECANE
129 PALMITANITRILE
130 1-HEXADECENE
131 N-HEXADECYL CHLORIDE
132 N-HEXADECYL BROMIDE
133 N-HEXADECANE
134 N-HEXADECANOL
135 N-OCTADECANE
136 N-EICOSANE
137 N-HENEICOSANE
138 N-TETRACOSANE
139 N-OCTACOSANE
140 SQUALENE
141 N-TRIACONTANE
142 N-SQUALANE
143 N-DOTRIACONTANE
144 N-PENTATRIACONTANE
145 N-UNDECANE
146 N-TRIDECANE

ID	COMPOUND
147	N-TETRADECANE
148	N-PENTADECANE
149	2-METHYLBUTANE
150	2-METHYLHEXANE
151	2,2,4-TRIMETHYLPENTANE
152	ADAMANTANE
153	1-BUTENE
154	CYCLOPENTENE
155	1-HEXYNE
156	1-HEPTYNE
157	1-PENTYNE
158	ETHYL CHLORIDE
159	1-CHLOROPROPANE
160	1-CHLOROBUTANE
161	1-CHLOROPENTANE
162	1-CHLOROHEXANE
163	1-CHLOROHEPTANE
164	METHYLENE CHLORIDE
165	1,1,2,2-TETRACHLOROETHANE
166	PENTACHLOROETHANE
167	TRANS-1,2-DICHLOROETHYLENE
168	TRICHLOROETHYLENE
169	TETRACHLOROETHYLENE
170	1,2-DIBROMOETHANE
171	FLOROTRICHLOROMETHANE
172	M-XYLENE
173	1,3,5-TRIMETHYLBENZENE
174	1,2,4-TRIMETHYLBENZENE
175	1,2,3-TRIMETHYLBENZENE
176	1,2,3,4-TETRAMETHYLBENZENE
177	1,2,3,5-TETRAMETHYLBENZENE
178	1,2,4,5-TETRAMETHYLBENZENE
179	PENTAMETHYLBENZENE
180	HEXAMETHYLBENZENE
181	N-PROPYLBENZENE
182	I-PROPYLBENZENE
183	T-BUTYL BENZENE
184	1-ISOPROPYL-4-METHYLBENZENE
185	T-AMYL BENZENE
186	FLUOROBENZENE
187	BROMOBENZENE
188	IODOBENZENE
189	1,2-DICHLOROBENZENE
190	1,3-DICHLOROBENZENE
191	1,4-DICHLOROBENZENE
192	1,2,3-TRICHLOROBENZENE
193	1,2,4-TRICHLOROBENZENE
194	1,3,5-TRICHLOROBENZENE
195	1,2,3,4-TETRACHLOROBENZENE

ID	COMPOUND
196	1,2,3,5-TETRACHLOROBENZENE
197	1,2,4,5-TETRACHLOROBENZENE
198	PENTACHLOROBENZENE
199	HEXACHLOROBENZENE
200	1,2-DIBROMOBENZENE
201	1,4-DIBROMOBENZENE
202	2-CHLOROTOLUENE
203	3-CHLOROTOLUENE
204	4-CHLOROTOLUENE
205	DIETHYL ETHER
206	DI(N-PROPYL)ETHER
207	DI(N-BUTYL)ETHER
208	DIISOPROPYL ETHER
209	TETRAHYDROPYRAN
210	ETHYL VINYL ETHER
211	2-METHYLANISOLE
212	3-METHYLANISOLE
213	4-METHYLANISOLE
214	4-CHLOROANISOLE
215	PHENETOLE
216	PHENYL PROPYL ETHER
217	METHYL 3-PHENYLETHYL ETHER
218	METHYL FORMATE
219	N-PENTYL ACETATE
220	ETHYL BUTYRATE
221	METHYL PENTANOATE
222	ETHYL PENTANOATE
223	METHYL HEXANOATE
224	ETHYL CHLOROACETATE
225	ETHYL TRICHLOROACETATE
226	METHYL ACRYLATE
227	ETHYL ACRYLATE
228	METHYL METHACRYLATE
229	METHYL BENZOATE
230	ETHYL BENZOATE
231	METHYL 2-METHYLBENZOATE
232	2-PHENYLETHYL ACETATE
233	3-PHENYLPROPYL ACETATE
234	METHYL PHENYLACETATE
235	ETHYL 3-PHENYLPROPINOATE
236	BENZYL BENZOATE
237	PHENYL ACETATE
238	2-METHYLPHENYL ACETATE
239	3-METHYLPHENYL ACETATE
240	4-METHYLPHENYL ACETATE
241	2-CHLOROPHENYL ACETATE
242	3-CHLOROPHENYL ACETATE
243	4-CHLOROPHENYL ACETATE
244	4-FLUOROPHENYL ACETATE

ID	COMPOUND
245	2-BROMOPHENYL ACETATE
246	ETHYL PHENOXYACETATE
247	ACETALDEHYDE
248	PROPIONALDEHYDE
249	BUTYRALDEHYDE
250	PENTANAL
251	HEXANAL
252	BENZALDEHYDE
253	TRANS-CROTONALDEHYDE
254	2-HEXANONE
255	2-HEPTANONE
256	CYCLOPENTANONE
257	3-CHLOROACETOPHENONE
258	4-CHLOROACETOPHENONE
259	4-BROMOACETOPHENONE
260	4-FLUOROACETOPHENONE
261	4-METHYLACETOPHENONE
262	PHENYLACETONE
263	4-PHENYL-2-BUTANONE
264	ETHYLAMINE
265	N-PROPYLAMINE
266	N-BUTYLAMINE
267	N-AMYLAMINE
268	N-HEXYLAMINE
269	N-HEPTYLAMINE
270	N-OCTYLAMINE
271	DIETHYLAMINE
272	DI(N-PROPYL)AMINE
273	DI(N-BUTYL)AMINE
274	TRIMETHYLAMINE
275	TRI(N-PROPYL)AMINE
276	O-TOLUIDINE
277	M-TOLUIDINE
278	P-TOLUIDINE
279	3-CHLOROANILINE
280	4-CHLOROANILINE
281	3-BROMOANILINE
282	4-BROMOANILINE
283	3-FLUOROANILINE
284	4-FLUOROANILINE
285	3-NITROANILINE
286	4-NITROANILINE
287	4-AMINOBIIPHENYL
288	4,4'-DIAMINOBIIPHENYL
289	1-NAPHTHYLAMINE
290	2-NAPHTHYLAMINE
291	N-METHYLANILINE
292	N-ETHYLANILINE
293	N,N-DIMETHYL ANILINE

ID	COMPOUND
294	N,N,4-TRIMETHYLANILINE
295	N,N-DIETHYLANILINE
296	BENZYLDIMETHYLAMINE
297	3-METHYLPYRIDINE
298	3-CHLOROPYRIDINE
299	4-CHLOROPYRIDINE
300	3-BROMOPYRIDINE
301	4-BROMOPYRIDINE
302	BUTYRONITRILE
303	PHENYLACETONITRILE
304	3-PHENYLPROPIONITRILE
305	ACRYLONITRILE
306	1-NITROBUTANE
307	1-NITROPENTANE
308	3-NITROTOLUENE
309	4-NITROTOLUENE
310	2-CHLORONITROBENZENE
311	3-CHLORONITROBENZENE
312	4-CHLORONITROBENZENE
313	3-BROMONITROBENZENE
314	4-BROMONITROBENZENE
315	1,3-DINITROBENZENE
316	1,4-DINITROBENZENE
317	N-BUTYL NITRATE
318	DIMETHYLACETAMIDE
319	DIETHYLACETAMIDE
320	BENZAMIDE
321	DIMETHYL SULFOXIDE
322	PHENYL METHYL SULFOXIDE
323	DIMETHYL SULFIDE
324	DIETHYL SULFIDE
325	BIS(CHLOROETHYL) SULFIDE
326	METHANETHIOL
327	ETHANETHIOL
328	1-BUTANETHIOL
329	2-METHYL-1-PROPANOL
330	2-METHYL-1-BUTANOL
331	3-METHYL-1-BUTANOL
332	2-METHYL-1-PENTANOL
333	4-METHYL-1-PENTANOL
334	2,2-DIMETHYL-1-BUTANOL
335	2-ETHYL-1-BUTANOL
336	1-HEPTANOL
337	2,2-DIMETHYL-1-PENTANOL
338	2-PROPEN-1-OL
339	4-PENTEN-1-OL
340	2-PROPANOL
341	2-BUTANOL
342	2-PENTANOL

ID	COMPOUND
343	3-PENTANOL
344	2-HEXANOL
345	3-HEXANOL
346	3-METHYL-2-PENTANOL
347	4-METHYL-2-PENTANOL
348	2-METHYL-3-PENTANOL
349	2-HEPTANOL
350	3-HEPTANOL
351	4-HEPTANOL
352	5-METHYL-2-HEXANOL
353	2-OCTANOL
354	3-PENTEN-2-OL
355	1-PENTEN-3-OL
356	1-HEXEN-3-OL
357	2-METHYL-2-PROPANOL
358	2-METHYL-2-BUTANOL
359	2-METHYL-2-PENTANOL
360	3-METHYL-3-PENTANOL
361	2-METHYL-2-HEXANOL
362	3-METHYL-3-HEXANOL
363	2-METHYL-2-HEPTANOL
364	3-METHYL-3-HEPTANOL
365	BENZYL ALCOHOL
366	3-METHYLBENZYL ALCOHOL
367	4-METHYLBENZYL ALCOHOL
368	3-CHLOROBENZYL ALCOHOL
369	4-CHLOROBENZYL ALCOHOL
370	2-PHENYLETHANOL
371	3-PHENYL-1-PROPANOL
372	2-PHENYL-2-PROPANOL
373	3-PHENYL-2-PROPEN-1-OL
374	M-CRESOL
375	P-CRESOL
376	3-CHLOROPHENOL
377	4-CHLOROPHENOL
378	3-BROMOPHENOL
379	4-BROMOPHENOL
380	3-FLUOROPHENOL
381	4-FLUOROPHENOL
382	1-NAPHTHOL
383	2-NAPHTHOL
384	FORMIC ACID
385	ACETIC ACID
386	PROPIONIC ACID
387	BUTYRIC ACID
388	PENTANOIC ACID
389	HEXANOIC ACID
390	DECANOIC ACID
391	BENZOIC ACID

ID	COMPOUND
392	3-METHYLBENZOIC ACID
393	4-METHYLBENZOIC ACID
394	3-CHLOROBENZOIC ACID
395	4-CHLOROBENZOIC ACID
396	3-BROMOBENZOIC ACID
397	4-BROMOBENZOIC ACID
398	3-FLUOROBENZOIC ACID
399	4-FLUOROBENZOIC ACID
400	PHENYLACETIC ACID
401	3-METHYLPHENYLACETIC ACID
402	3-CHLOROPHENYLACETIC ACID
403	4-CHLOROPHENYLACETIC ACID
404	3-BROMOPHENYLACETIC ACID
405	2-FLUOROPHENYLACETIC ACID
406	3-FLUOROPHENYLACETIC ACID
407	4-FLUOROPHENYLACETIC ACID
408	3-PHENYLPROPIONIC ACID
409	4-PHENYLBUTANOIC ACID
410	1-NAPHTHALENECARBOXYLIC ACID
411	NAPHTHALENE
412	1-METHYLNAPHTHALENE
413	2-METHYLNAPHTHALENE
414	1,3-DIMETHYLNAPHTHALENE
415	1,4-DIMETHYLNAPHTHALENE
416	1,5-DIMETHYLNAPHTHALENE
417	2,3-DIMETHYLNAPHTHALENE
418	2,6-DIMETHYLNAPHTHALENE
419	1-ETHYLNAPHTHALENE
420	1,4,5-TRIMETHYLNAPHTHALENE
421	1-CHLORONAPHTHALENE
422	2-CHLORONAPHTHALENE
423	1-NITRONAPHTHALENE
424	ANTHRACENE
425	2-METHYLANTHRACENE
426	9-METHYLANTHRACENE
427	9,10-DIMETHYLANTHRACENE
428	PHENANTHRENE
429	2-METHYLPHENANTHRENE
430	2-CHLOROPHENANTHRENE
431	BENZ[A]ANTHRACENE
432	1-METHYLBENZ[A]ANTHRACENE
433	7-METHYLBENZ[A]ANTHRACENE
434	12-METHYLBENZ[A]ANTHRACENE
435	7,12-DIMETHYLBENZ[A]ANTHRACENE
436	7-ETHYLBENZ[A]ANTHRACENE
437	BENZ[B]ANTHRACENE
438	CHRYSENE
439	5-METHYLCHRYSENE
440	6-METHYLCHRYSENE

ID	COMPOUND
441	5,6-DIMETHYLCHRYSENE
442	TRIPHENYLENE
443	DIBENZ[AH]ANTHRACENE
444	DIBENZ[AJ]ANTHRACENE
445	PYRENE
446	BENZO[A]PYRENE
447	BENZO[E]PYRENE
448	6-METHYLBENZO[E]PYRENE
449	PERYLENE
450	BENZO[GHI]PERYLENE
451	FLOURENE
452	1-METHYLFLUORENE
453	BENZO[A]FLUORENE
454	BENZO[B]FLUORENE
455	ACENAPHTHENE
456	FLUORANTHENE
457	BENZO[B]FLUORANTHENE
458	BENZO[J]FLUORANTHENE
459	BENZO[K]FLUORANTHENE
460	CHOLANTHRENE
461	3-METHYLCHOLANTHRENE
462	ISOQUINOLINE
463	1-METHYLISOQUINOLINE
464	BENZO[F]QUINOLINE
465	ACRIDINE
466	DIBENZ[AH]ACRIDINE
467	2,2'-BIQUINOLINE
468	BIPHENYL
469	2-CHLORO BIPHENYL
470	2,4'-DICHLOROBIPHENYL
471	2,5-DICHLOROBIPHENYL
472	2,6-DICHLOROBIPHENYL
473	2,2',4-TRICHLOROBIPHENYL
474	2,4,5-TRICHLOROBIPHENYL
475	2,4,6-TRICHLOROBIPHENYL
476	2,2',4,5-TETRACHLOROBIPHENYL
477	2,3,4,5-TETRACHLOROBIPHENYL
478	2,2',4,5,5'-PENTACHLOROBIPHENYL
479	2,3,4,5,6-PENTACHLOROBIPHENYL
480	2,2',3,3',4,4'-HEXACHLOROBIPHENYL
481	2,2',3,3',6,6'-HEXACHLOROBIPHENYL
482	2,3,4,4',5,6-HEXACHLOROBIPHENYL
483	2,2',4,4',6,6'-HEXACHLOROBIPHENYL
484	2,2',3,3',4,4',6-HEPTACHLOROBIPHENYL
485	2,2',3,3',5,5',6,6'-OCTACHLOROBIPHENYL
486	2,2',3,3',4,5,5',6,6'-NONACHLOROBIPHENYL
487	PERCHLORO BIPHENYL
488	1,2-DIPHENYLETHANE
489	PERFLUOROHXANE

ID	COMPOUND
490	TRICHLOROMETHANE
491	DIMETHYL KETONE
492	2,2,2-TRIFLUOROETHANOL
493	N,N-DIMETHYL FORMAMIDE
494	FORMAMIDE
495	WATER
496	1,1,1,3,3,3-HEXAFLUORO-2-PROPANOL
497	1,1,1-TRICHLOROACETONE
498	N,N-DIMETHYL TRIFLUOROACETAMIDE
499	ETHYL-1,1,1-TRIFLUOROETHANOATE
500	ETHYL-1,1,1-TRICHLOROETHANOATE
501	METHYL DIMETHYLCARBAMATE
502	1-METHYL-2-PYRROLIDINONE (NMP)
503	1,1,3,3-TETRAMETHYL UREA
504	2,6-DIMETHYL-GAMMA-PYRONE
505	3-DIETHYLAMINO-5,5-DIMETHYLCYCLOHEX-2-ENONE
506	ACETIC ANHYDRIDE
507	BIS(2-METHOXYETHYL)ETHER
508	CUMENE
509	M-DICHLOROBENZENE
510	ETHYL ACETOACETATE
511	3-HEPTANONE
512	2,6-LUTIDINE
513	METHYLAL
514	TRIMETHYL ORTHOACETATE
515	TRIMETHYL ORTHOFORMATE
516	PERFLUORO HEPTANE
517	PERFLUORO OCTANE
518	MESITYLENE
519	VALERONITRILE
520	HEXYL CYANIDE
521	HEPTYL CYANIDE
522	OCTYL CYANIDE
523	NONYL CYANIDE
524	TETRADECYL CYANIDE
525	1,2-DIMETHOXY ETHER
526	DIPHENYL ETHER
527	BUTYROLACTONE
528	BUTYL ACETATE
529	DIETHYL MALONATE
530	PROPYLENE CARBONATE
531	TRIBUTYL AMINE
532	SULFOLANE
533	BUTYL CHLORIDE
534	OV-101
535	OV-3
536	OV-7
537	OV-11
538	OV-17

ID COMPOUND
539 OV-22
540 OV-25
541 PROPYL CHLORIDE
542 ETHYLENE GLYCOL
543 DIBENZYL ETHER
544 DICYCLOPROPYL KETONE
545 METHYL CYCLOPROPYL KETONE
546 TETRAMETHYL UREA
547 TRIFLUORO ACETIC ACID
548 ETHYL SULFATE
549 TRIETHYL PHOSPHATE
550 4-METHYL PYRIDINE
551 2,6-DIMETHYL PYRIDINE
552 METHYLENE BROMIDE
553 METHYLENE IODIDE
554 T-BUTANOL
555 TRIFLUORO ETHANOL
556 HEXAFLUORO ISOPROPANOL
557 2-FLUORO ETHANOL
558 2-METHOXY ETHANOL
559 METHYL ETHYL KETONE
560 N,N-DIMETHYL ACETAMIDE
561 N-METHYL PYRROLIDONE
562 HEXAMETHYL PHOSPHORAMIDE
563 METHYL T-BUTYL KETONE
564 DIMETHYL-(GAMMA)-PYRONE
565 BENZOPHENONE
566 BIACETYL
567 SYM-DICHLOROACETONE
568 P-METHOXYACETOPHENONE
569 ACETYLFERROCENE
570 FLAVONE
571 P-NITROBENZALDEHYDE
572 P-CHLOROBENZALDEHYDE
573 P-METHOXYBENZALDEHYDE
574 P-(DIMETHYLAMINO)BENZALDEHYDE
575 2-NAPHTHALDEHYDE
576 DI(T-BUTYL)KETONE
577 CINNAMALDEHYDE
578 ISOBUTYROPHENONE
579 P-CHLOROACETOPHENONE
580 P-METHYLACETOPHENONE
581 DIETHYL CARBONATE
582 METHYL TRIFLUORO ACETATE
583 PHENYL BENZOATE
584 ETHYL P-NITRO BENZOATE
585 DIMETHYL CARBONATE
586 ETHYL TRIFLUOROACETATE
587 N,N-DIMETHYL CHLOROACETAMIDE

ID COMPOUND
588 N,N-DIMETHYL-P-NITROBENZAMIDE
589 N,N-DIMETHYL BENZAMIDE
590 N,N-DI-N-HEXYLACETAMIDE
591 N,N-DIETHYL ACETAMIDE
592 N,N-DIETHYL BENZAMIDE
593 N-ACETYL PIPERIDINE
594 N,N-DIPHENYL ACETAMIDE
595 TETRAETHYL UREA
596 N-METHYL PYRIDONE
597 ETHYL DIETHYLCARBAMATE
598 N,N-DIETHYLPROPIONAMIDE
599 N,N-DIPHENYLPROPIONAMIDE
600 BENZOYL FLUORIDE
601 PROPIONYL FLUORIDE
602 BENZOYL CHLORIDE
603 BENZOYL BROMIDE
604 TRI(N-BUTYL)AMINE
605 N,N-DIMETHYL BENZYLAMINE
606 TRIALLYLAMINE
607 N,N-DIMETHYL-N-PROPYLAMINE
608 N,N-DIMETHYL-N-CYCLOHEXYLAMINE
609 B,B,B-TRIFLUOROETHYLAMINE
610 PROPARGYLAMINE
611 CYCLOPROPYLAMINE
612 BENZYLAMINE
613 QUINUCLIDINE
614 N-METHYLIMIDAZOLE
615 1,4-DIAZABICYCLO[2,2,2]OCTANE (DABCO)
616 DIPHENYL SULFOXIDE
617 DI(N-BUTYL)SULFOXIDE
618 METHYL PHENYL SULFOXIDE
619 METHYL P-NITROPHENYL SULFOXIDE
620 DIETHYL SULFITE
621 DI(N-PROPYL)SULFITE
622 DI(N-BUTYL)SULFITE
623 DI(P-TOLYL)SULFOXIDE
624 DIISOPROPYL SULFOXIDE
625 TETRAMETHYLENE SULFOXIDE
626 HEXAMETHYLPHOSPHORAMIDE
627 TRI(N-BUTYL)PHOSPHATE
628 TRIPHENYLPHOSPHINE OXIDE
629 TRIMETHYL PHOSPHATE
630 TRIMETHYLPHOSPHINE OXIDE
631 TRIPHENYL PHOSPHINATE
632 DIETHOXY(TRICHLOROMETHYL)PHOSPHINE OXIDE
633 DIETHOXY(DICHLOROMETHYL)PHOSPHINE OXIDE
634 DIETHOXY(CHLOROMETHYL)PHOSPHINE OXIDE
635 DIMETHOXYPHOSPHINE OXIDE
636 DIETHOXYPHOSPHINE OXIDE

ID COMPOUND
637 DIISOPROPOXYPHOSPHINE OXIDE
638 DIMETHOXYETHYLPHOSPHINE OXIDE
639 DIETHOXYMETHYLPHOSPHINE OXIDE
640 DIETHOXY(DIMETHYLAMINO)PHOSPHINE OXIDE
641 TRI(N-PROPYL)PHOSPHINE OXIDE
642 TRIETHYLPHOSPHINE OXIDE
643 P-METHOXYBENZONITRILE
644 B-ETHOXYPROPIONITRILE
645 P-(DIMETHYLAMINO)BENZONITRILE
646 2,4,6-TRIMETHYL PYRIDINE
647 3,5-DICHLOROPYRIDINE
648 4-(DIMETHYLAMINO)PYRIDINE
649 2-N-BUTYLPYRIDINE
650 PYRIMIDINE
651 2,4-DIMETHYLPYRIDINE
652 4-METHOXPYRIDINE
653 O-DICHLOROBENZENE
654 PERFLUORODIMETHYLDECALIN
655 PERFLUOROTRI-N-BUTYLAMINE

**-A34-
ALKANES**

- 30 N-PROPANE
- 42 N-BUTANE
- 47 CYCLOPENTANE
- 61 N-PENTANE
- 62 ISOPENTANE
- 72 CYCLOHEXANE
- 75 METHYL CYCLOPENTANE
- 80 N-HEXANE
- 81 2,3-DIMETHYL BUTANE
- 82 3-METHYL PENTANE
- 83 2,2-DIMETHYL BUTANE
- 84 2,4-DIMETHYL PENTANE
- 85 2-METHYL PENTANE
- 94 METHYL CYCLOHEXANE
- 96 CYCLOHEPTANE
- 98 N-HEPTANE
- 99 3-METHYL HEXANE
- 100 2,2-DIMETHYLPENTANE
- 105 CYCLOOCTANE
- 107 ETHYL CYCLOHEXANE
- 108 ISOCTANE
- 109 N-OCTANE
- 114 1,3,5-TRIMETHYLCYCLOHEXANE
- 117 N-NONANE
- 123 BUTYL CYCLOHEXANE
- 126 N-DECANE
- 128 N-DODECANE
- 133 N-TRIDECANE
- 135 N-HEXADECANE
- 136 N-HEPTADECANE
- 137 N-OCTADECANE
- 138 N-ICOSANE
- 137 N-HENEICOSANE
- 138 N-TETRACOSANE
- 139 N-OCTACOSANE
- 141 N-TRIACONTANE
- 142 N-SQUALANE
- 143 N-DOTRIACONTANE
- 144 N-PENTATRIACONTANE

GAMMA INFINITY OVERALL DATABASE

SLT	SLV		TEMP	GAMMA	REF
ID	ID	SOLVENT		INF.	
4	108	ISOOCTANE	293.14	1.51	2
19	88	BENZONITRILE	293.15	4.70	2
18	88	BENZONITRILE	293.15	1.33	2
98	88	BENZONITRILE	293.15	7.53	2
17	88	BENZONITRILE	293.15	1.58	2
61	88	BENZONITRILE	293.15	6.08	2
10	88	BENZONITRILE	293.15	1.41	2
48	88	BENZONITRILE	293.15	3.10	2
8	88	BENZONITRILE	293.15	4.70	4
80	88	BENZONITRILE	293.15	6.68	2
6	88	BENZONITRILE	293.15	0.70	2
50	88	BENZONITRILE	293.15	3.62	2
72	88	BENZONITRILE	293.15	4.92	2
46	88	BENZONITRILE	293.15	2.12	2
1	88	BENZONITRILE	293.15	2.33	2
40	91	TOLUENE	293.15	1.19	2
28	91	TOLUENE	293.15	1.05	2
4	91	TOLUENE	293.15	0.67	2
36	91	TOLUENE	293.15	1.28	2
2	91	TOLUENE	293.15	1.02	2
1	91	TOLUENE	293.15	1.27	2
9	91	TOLUENE	293.15	4.41	2
46	91	TOLUENE	293.15	1.18	2
11	91	TOLUENE	293.15	4.00	2
48	91	TOLUENE	293.15	1.37	2
18	91	TOLUENE	293.15	0.98	2
50	91	TOLUENE	293.15	1.44	2
21	91	TOLUENE	293.15	1.98	2
61	91	TOLUENE	293.15	1.80	2
8	91	TOLUENE	293.15	23.10	2
72	91	TOLUENE	293.15	1.59	2
17	91	TOLUENE	293.15	1.06	2
80	91	TOLUENE	293.15	1.74	2
6	91	TOLUENE	293.15	0.85	2
19	91	TOLUENE	293.15	18.40	2
10	91	TOLUENE	293.15	1.15	2
87	91	TOLUENE	293.15	1.21	2
1	92	ANISOLE	293.15	1.62	2
36	92	ANISOLE	293.15	1.08	2
2	92	ANISOLE	293.15	1.30	2
46	92	ANISOLE	293.15	1.54	2
6	92	ANISOLE	293.15	0.77	2
48	92	ANISOLE	293.15	2.25	2
10	92	ANISOLE	293.15	1.14	2
50	92	ANISOLE	293.15	2.43	2
17	92	ANISOLE	293.15	1.12	2

SLT	SLV	SOLVENT	TEMP	GAMMA	REF
ID	ID			INF.	
61	92	ANISOLE	293.15	3.64	2
19	92	ANISOLE	293.15	10.00	2
66	92	ANISOLE	293.15	1.05	2
4	92	ANISOLE	293.15	0.68	2
72	92	ANISOLE	293.15	3.10	2
11	92	ANISOLE	293.15	2.26	2
80	92	ANISOLE	293.15	3.94	2
28	92	ANISOLE	293.15	1.14	2
18	92	ANISOLE	293.15	1.08	2
8	92	ANISOLE	293.15	11.00	2
98	92	ANISOLE	293.15	4.25	2
18	98	N-HEPTANE	293.15	1.62	2
17	98	N-HEPTANE	293.15	1.90	2
40	98	N-HEPTANE	293.15	1.44	2
46	98	N-HEPTANE	293.15	1.03	2
28	98	N-HEPTANE	293.15	1.47	2
1	98	N-HEPTANE	293.15	1.30	2
18	101	ACETOPHENONE	293.15	1.18	2
46	101	ACETOPHENONE	293.15	1.92	2
2	101	ACETOPHENONE	293.15	1.70	2
48	101	ACETOPHENONE	293.15	2.82	2
6	101	ACETOPHENONE	293.15	0.62	2
50	101	ACETOPHENONE	293.15	3.88	2
10	101	ACETOPHENONE	293.15	1.23	2
61	101	ACETOPHENONE	293.15	6.00	2
1	101	ACETOPHENONE	293.15	2.05	2
72	101	ACETOPHENONE	293.15	4.40	2
28	101	ACETOPHENONE	293.15	1.39	2
80	101	ACETOPHENONE	293.15	6.84	2
8	101	ACETOPHENONE	293.15	3.47	2
94	101	ACETOPHENONE	293.15	4.63	2
19	101	ACETOPHENONE	293.15	3.62	2
17	101	ACETOPHENONE	293.15	1.42	2
4	101	ACETOPHENONE	293.15	0.58	2
98	101	ACETOPHENONE	293.15	7.58	2
28	103	P-XYLENE	293.15	1.03	2
40	103	P-XYLENE	293.15	1.24	2
46	103	P-XYLENE	293.15	1.03	2
6	103	P-XYLENE	293.15	0.85	2
48	103	P-XYLENE	293.15	1.19	2
11	103	P-XYLENE	293.15	5.05	2
50	103	P-XYLENE	293.15	1.24	2
18	103	P-XYLENE	293.15	1.00	2
61	103	P-XYLENE	293.15	1.48	2
1	103	P-XYLENE	293.15	1.07	2
66	103	P-XYLENE	293.15	0.99	2
87	103	P-XYLENE	293.15	1.08	2
2	103	P-XYLENE	293.15	0.93	2

SLT	SLV		TEMP	GAMMA	REF
ID	ID	SOLVENT		INF	
17	103	P-XYLENE	293.15	1.03	2
72	103	P-XYLENE	293.15	1.35	2
36	103	P-XYLENE	293.15	1.33	2
21	103	P-XYLENE	293.15	2.13	2
10	103	P-XYLENE	293.15	1.06	2
80	103	P-XYLENE	293.15	1.44	2
1	108	ISOOCTANE	293.15	1.33	2
19	108	ISOOCTANE	293.15	46.00	2
20	108	ISOOCTANE	293.15	20.00	2
6	108	ISOOCTANE	293.15	2.13	2
21	108	ISOOCTANE	293.15	7.15	2
9	108	ISOOCTANE	293.15	38.50	2
28	108	ISOOCTANE	293.15	1.47	2
11	108	ISOOCTANE	293.15	31.50	2
32	108	ISOOCTANE	293.15	3.86	2
17	108	ISOOCTANE	293.15	1.87	2
36	108	ISOOCTANE	293.15	3.12	2
61	108	ISOOCTANE	293.15	0.98	2
46	108	ISOOCTANE	293.15	0.98	2
10	108	ISOOCTANE	293.15	1.95	2
48	108	ISOOCTANE	293.15	0.97	2
18	108	ISOOCTANE	293.15	1.63	2
16	108	ISOOCTANE	293.15	18.90	2
8	108	ISOOCTANE	293.15	78.00	2
50	108	ISOOCTANE	293.15	0.99	2
32	109	N-OCTANE	293.15	4.15	2
50	109	N-OCTANE	293.15	0.98	2
18	109	N-OCTANE	293.15	1.82	2
19	109	N-OCTANE	293.15	50.50	2
61	109	N-OCTANE	293.15	0.97	2
20	109	N-OCTANE	293.15	20.90	2
8	109	N-OCTANE	293.15	80.00	2
21	109	N-OCTANE	293.15	7.30	2
10	109	N-OCTANE	293.15	1.86	2
28	109	N-OCTANE	293.15	1.47	2
14	109	N-OCTANE	293.15	2.90	2
34	109	N-OCTANE	293.15	1.50	2
17	109	N-OCTANE	293.15	1.80	2
36	109	N-OCTANE	293.15	3.25	2
6	109	N-OCTANE	293.15	2.15	2
46	109	N-OCTANE	293.15	0.99	2
11	109	N-OCTANE	293.15	31.30	2
48	109	N-OCTANE	293.15	0.94	2
1	109	N-OCTANE	293.15	1.26	2
16	109	N-OCTANE	293.15	19.10	2
9	109	N-OCTANE	293.15	39.60	2
4	109	N-OCTANE	293.15	1.43	2
46	110	N-OCTANOL	293.15	1.90	2

SLT ID	SLV ID	SOLVENT	TEMP	GAMMA INF.	REF
14	110	N-OCTANOL	293.15	2.33	2
2	110	N-OCTANOL	293.15	1.74	2
11	110	N-OCTANOL	293.15	7.48	2
1	110	N-OCTANOL	293.15	1.75	2
10	110	N-OCTANOL	293.15	2.06	2
4	110	N-OCTANOL	293.15	0.95	2
21	110	N-OCTANOL	293.15	2.57	2
18	110	N-OCTANOL	293.15	1.99	2
6	110	N-OCTANOL	293.15	1.56	2
36	110	N-OCTANOL	293.15	2.37	2
20	110	N-OCTANOL	293.15	6.34	2
28	110	N-OCTANOL	293.15	2.10	2
32	110	N-OCTANOL	293.15	2.02	2
17	110	N-OCTANOL	293.15	2.29	2
9	110	N-OCTANOL	293.15	10.40	2
19	89	BENZYL CHLORIDE	293.20	12.10	2
61	89	BENZYL CHLORIDE	293.20	4.10	2
50	89	BENZYL CHLORIDE	293.20	2.62	2
18	89	BENZYL CHLORIDE	293.20	1.03	2
10	89	BENZYL CHLORIDE	293.20	1.09	2
8	89	BENZYL CHLORIDE	293.20	13.90	2
6	89	BENZYL CHLORIDE	293.20	0.85	2
48	89	BENZYL CHLORIDE	293.20	2.28	2
80	89	BENZYL CHLORIDE	293.20	4.40	2
1	89	BENZYL CHLORIDE	293.20	1.60	2
46	89	BENZYL CHLORIDE	293.20	1.90	2
40	89	BENZYL CHLORIDE	293.20	1.48	2
4	89	BENZYL CHLORIDE	293.20	0.83	2
28	89	BENZYL CHLORIDE	293.20	1.22	2
20	91	TOLUENE	293.20	2.64	2
8	98	N-HEPTANE	293.20	80.00	2
20	98	N-HEPTANE	293.20	21.90	2
36	98	N-HEPTANE	293.20	3.29	2
72	98	N-HEPTANE	293.20	0.99	2
39	98	N-HEPTANE	293.20	1.50	2
6	98	N-HEPTANE	293.20	2.20	1
50	98	N-HEPTANE	293.20	0.98	2
9	98	N-HEPTANE	293.20	41.00	2
11	98	N-HEPTANE	293.20	30.00	2
80	98	N-HEPTANE	293.20	1.00	2
16	98	N-HEPTANE	293.20	19.80	1
48	98	N-HEPTANE	293.20	0.97	2
4	98	N-HEPTANE	293.20	1.47	1
61	98	N-HEPTANE	293.20	0.99	2
14	98	N-HEPTANE	293.20	3.30	2
10	98	N-HEPTANE	293.20	1.94	2
19	98	N-HEPTANE	293.20	51.00	1
2	98	N-HEPTANE	293.20	1.20	2

SLT	SLV		TEMP	GAMMA	REF
ID	ID	SOLVENT		INF.	
11	101	ACETOPHENONE	293.20	1.65	2
21	133	N-HEXADECANE	293.20	6.30	58
20	80	N-HEXANE	295.00	19.20	1
11	80	N-HEXANE	295.00	27.60	1
44	80	N-HEXANE	296.60	5.90	1
87	80	N-HEXANE	298.00	1.10	1
14	80	N-HEXANE	298.00	3.17	1
32	80	N-HEXANE	298.00	4.38	1
70	80	N-HEXANE	298.00	7.10	1
17	80	N-HEXANE	298.00	2.07	1
16	80	N-HEXANE	298.10	20.70	1
36	80	N-HEXANE	298.10	3.39	1
19	87	TRIETHYLAMINE	298.15	1.82	4
66	90	BROMOANISOLE	298.15	1.14	2
40	90	BROMOANISOLE	298.15	1.84	2
72	90	BROMOANISOLE	298.15	3.02	2
36	90	BROMOANISOLE	298.15	1.19	2
4	90	BROMOANISOLE	298.15	0.43	2
14	90	BROMOANISOLE	298.15	1.13	2
11	90	BROMOANISOLE	298.15	2.75	2
17	90	BROMOANISOLE	298.15	1.28	2
80	90	BROMOANISOLE	298.15	4.26	2
18	90	BROMOANISOLE	298.15	1.20	2
10	90	BROMOANISOLE	298.15	1.23	2
2	90	BROMOANISOLE	298.15	1.50	2
21	90	BROMOANISOLE	298.15	1.39	2
46	90	BROMOANISOLE	298.15	1.78	2
40	111	QUINOLINE	298.15	2.39	2
18	111	QUINOLINE	298.15	1.27	2
4	111	QUINOLINE	298.15	0.47	2
36	111	QUINOLINE	298.15	1.49	2
17	111	QUINOLINE	298.15	1.55	2
66	111	QUINOLINE	298.15	1.32	2
14	111	QUINOLINE	298.15	0.92	2
72	111	QUINOLINE	298.15	4.35	2
11	111	QUINOLINE	298.15	2.14	2
46	111	QUINOLINE	298.15	2.43	2
2	111	QUINOLINE	298.15	1.44	2
21	111	QUINOLINE	298.15	1.50	2
10	111	QUINOLINE	298.15	1.25	2
80	111	QUINOLINE	298.15	6.50	2
10	112	PROPIOPHENONE	298.15	1.21	2
40	113	BENZYL ACETATE	298.15	1.68	2
21	113	BENZYL ACETATE	298.15	1.12	2
18	113	BENZYL ACETATE	298.15	1.02	2
72	113	BENZYL ACETATE	298.15	3.45	2
17	113	BENZYL ACETATE	298.15	1.32	2
46	113	BENZYL ACETATE	298.15	1.68	2

SLT	SLV	SOLVENT	TEMP	GAMMA	REF
ID	ID			INF.	
14	113	BENZYL ACETATE	298.15	0.71	2
36	113	BENZYL ACETATE	298.15	1.00	2
11	113	BENZYL ACETATE	298.15	1.51	2
80	113	BENZYL ACETATE	298.15	5.28	2
10	113	BENZYL ACETATE	298.15	1.13	2
2	113	BENZYL ACETATE	298.15	1.41	2
66	113	BENZYL ACETATE	298.15	1.04	2
28	113	BENZYL ACETATE	298.15	1.22	2
4	113	BENZYL ACETATE	298.15	0.51	2
17	119	BROMONAPHTHALENE	298.15	1.22	2
4	119	BROMONAPHTHALENE	298.15	1.13	2
40	119	BROMONAPHTHALENE	298.15	2.14	2
21	119	BROMONAPHTHALENE	298.15	2.13	2
10	119	BROMONAPHTHALENE	298.15	1.24	2
18	119	BROMONAPHTHALENE	298.15	1.23	2
14	119	BROMONAPHTHALENE	298.15	1.43	2
36	119	BROMONAPHTHALENE	298.15	1.82	2
66	119	BROMONAPHTHALENE	298.15	1.39	2
80	119	BROMONAPHTHALENE	298.15	4.90	2
2	119	BROMONAPHTHALENE	298.15	1.57	2
28	119	BROMONAPHTHALENE	298.15	1.49	2
46	119	BROMONAPHTHALENE	298.15	2.06	2
11	119	BROMONAPHTHALENE	298.15	4.40	2
72	119	BROMONAPHTHALENE	298.15	2.80	2
109	80	N-HEXANE	298.20	1.02	4
37	80	N-HEXANE	298.20	4.12	4
87	80	N-HEXANE	298.20	1.00	9
32	80	N-HEXANE	298.20	4.19	4
91	80	N-HEXANE	298.20	1.67	1
9	87	TRIETHYLAMINE	298.20	8.95	4
32	87	TRIETHYLAMINE	298.20	2.08	4
37	87	TRIETHYLAMINE	298.20	2.24	4
91	87	TRIETHYLAMINE	298.20	1.05	4
87	88	BENZONITRILE	298.20	2.84	9
28	90	BROMOANISOLE	298.20	1.41	2
37	91	TOLUENE	298.20	1.25	4
32	91	TOLUENE	298.20	1.37	4
109	91	TOLUENE	298.20	1.44	4
9	92	ANISOLE	298.20	1.86	4
32	92	ANISOLE	298.20	1.01	4
109	92	ANISOLE	298.20	4.96	4
37	92	ANISOLE	298.20	0.96	4
91	92	ANISOLE	298.20	1.43	4
19	92	ANISOLE	298.20	6.72	4
66	93	HEPTANENITRILE	298.20	0.90	32
48	93	HEPTANENITRILE	298.20	1.87	32
46	93	HEPTANENITRILE	298.20	1.30	32
80	93	HEPTANENITRILE	298.20	3.01	32

SLT	SLV	SOLVENT	TEMP	GAMMA	INF.	REF
10	10	SOLVENT				
72	99	HEPTANENITRILE	298.20	2.59		32
87	98	N-HEPTANE	298.20	1.00		9
48	101	ACETOPHENONE	298.20	3.06		36
80	101	ACETOPHENONE	298.20	6.08		36
46	101	ACETOPHENONE	298.20	2.05		36
98	101	ACETOPHENONE	298.20	6.82		36
87	101	ACETOPHENONE	298.20	3.07		9
66	101	ACETOPHENONE	298.20	1.20		36
37	101	ACETOPHENONE	298.20	0.92		4
61	101	ACETOPHENONE	298.20	5.37		36
32	101	ACETOPHENONE	298.20	1.02		4
66	101	ACETOPHENONE	298.20	1.24		32
91	101	ACETOPHENONE	298.20	1.44		4
80	101	ACETOPHENONE	298.20	6.74		32
109	101	ACETOPHENONE	298.20	8.86		4
72	101	ACETOPHENONE	298.20	4.34		36
19	101	ACETOPHENONE	298.20	2.55		4
91	103	P-XYLENE	298.20	1.03		4
109	103	P-XYLENE	298.20	1.81		4
91	108	ISOOCTANE	298.20	1.48		4
37	108	ISOOCTANE	298.20	3.61		4
32	108	ISOOCTANE	298.20	3.83		4
91	110	N-OCTANOL	298.20	2.19		4
9	110	N-OCTANOL	298.20	8.52		4
37	110	N-OCTANOL	298.20	2.20		4
32	110	N-OCTANOL	298.20	1.94		4
28	111	QUINOLINE	298.20	1.59		2
109	111	QUINOLINE	298.20	9.02		4
37	111	QUINOLINE	298.20	1.21		4
66	112	PROPIOPHENONE	298.20	1.07		2
14	112	PROPIOPHENONE	298.20	0.83		2
80	112	PROPIOPHENONE	298.20	4.57		2
36	112	PROPIOPHENONE	298.20	1.30		2
46	112	PROPIOPHENONE	298.20	1.70		2
2	112	PROPIOPHENONE	298.20	1.53		2
72	112	PROPIOPHENONE	298.20	3.41		2
40	112	PROPIOPHENONE	298.20	1.73		2
305	112	PROPIOPHENONE	298.20	1.80		2
21	112	PROPIOPHENONE	298.20	1.31		2
28	112	PROPIOPHENONE	298.20	1.29		2
18	112	PROPIOPHENONE	298.20	1.09		2
4	112	PROPIOPHENONE	298.20	0.54		2
17	112	PROPIOPHENONE	298.20	1.35		2
80	121	DECALIN	298.20	1.26		32
109	126	N-DECANE	298.20	1.08		4
91	126	N-DECANE	298.20	1.30		4
37	126	N-DECANE	298.20	3.30		4
32	126	N-DECANE	298.20	3.79		4

SLT	SLV	SOLVENT	TEMP	GAMMA	REF
ID	ID			INF.	
19	133	N-HEXADECANE	298.20	47.00	58
61	133	N-HEXADECANE	298.20	0.89	58
32	133	N-HEXADECANE	298.20	3.80	58
62	133	N-HEXADECANE	298.20	0.89	60
22	133	N-HEXADECANE	298.20	3.70	58
61	133	N-HEXADECANE	298.20	0.83	60
98	133	N-HEXADECANE	298.20	0.93	60
80	133	N-HEXADECANE	298.20	0.89	60
6	133	N-HEXADECANE	298.20	71.50	58
80	133	N-HEXADECANE	298.20	0.90	37
85	133	N-HEXADECANE	298.20	0.85	58
75	133	N-HEXADECANE	298.20	0.71	58
31	133	N-HEXADECANE	298.20	31.50	58
23	133	N-HEXADECANE	298.20	3.60	58
82	133	N-HEXADECANE	298.20	0.84	60
109	133	N-HEXADECANE	298.20	0.99	60
85	133	N-HEXADECANE	298.20	0.91	60
21	133	N-HEXADECANE	298.20	6.30	58
83	133	N-HEXADECANE	298.20	0.91	60
83	133	N-HEXADECANE	298.20	0.94	58
81	133	N-HEXADECANE	298.20	0.85	60
36	133	N-HEXADECANE	298.20	2.80	58
32	142	N-SQUALANE	298.20	2.03	4
109	142	N-SQUALANE	298.20	0.69	4
91	142	N-SQUALANE	298.20	0.70	4
31	80	N-HEXANE	301.00	39.00	1
4	80	N-HEXANE	301.00	1.58	1
18	80	N-HEXANE	301.00	1.62	1
39	80	N-HEXANE	301.00	1.52	1
2	80	N-HEXANE	301.00	1.20	1
72	80	N-HEXANE	301.00	1.09	1
43	80	N-HEXANE	301.00	33.00	1
24	80	N-HEXANE	301.00	14.10	1
40	80	N-HEXANE	301.00	1.45	1
73	88	BENZONITRILE	303.20	3.73	38
80	88	BENZONITRILE	303.20	5.90	38
69	88	BENZONITRILE	303.20	2.58	38
72	88	BENZONITRILE	303.20	4.41	38
66	88	BENZONITRILE	303.20	1.17	38
47	126	N-DECANE	303.20	0.87	58
66	126	N-DECANE	303.20	1.23	58
47	133	N-HEXADECANE	303.20	0.74	58
83	133	N-HEXADECANE	303.20	0.93	58
62	133	N-HEXADECANE	303.20	0.92	58
61	133	N-HEXADECANE	303.20	0.88	58
85	133	N-HEXADECANE	303.20	0.91	58
66	142	N-SQUALANE	303.20	0.65	58
61	142	N-SQUALANE	303.20	0.59	58

SLT	SLV		TEMP	GAMMA	REF
ID	ID	SOLVENT		INF.	
80	142	N-SQUALANE	303.20	0.61	58
98	142	N-SQUALANE	303.20	0.67	58
72	142	N-SQUALANE	303.20	0.49	58
83	142	N-SQUALANE	303.20	0.61	58
19	80	N-HEXANE	304.80	38.00	1
34	80	N-HEXANE	304.80	1.65	1
91	80	N-HEXANE	304.80	1.59	1
109	135	N-OCTADECANE	308.20	0.91	65
98	135	N-OCTADECANE	308.20	0.89	65
42	135	N-OCTADECANE	308.20	0.88	65
95	135	N-OCTADECANE	308.20	0.89	65
72	135	N-OCTADECANE	308.20	0.76	65
85	135	N-OCTADECANE	308.20	0.91	65
62	135	N-OCTADECANE	308.20	0.90	65
83	135	N-OCTADECANE	308.20	0.94	65
50	135	N-OCTADECANE	308.20	0.88	65
66	135	N-OCTADECANE	308.20	0.99	65
81	135	N-OCTADECANE	308.20	0.88	65
106	135	N-OCTADECANE	308.20	0.92	65
73	135	N-OCTADECANE	308.20	0.89	65
82	135	N-OCTADECANE	308.20	0.88	65
84	135	N-OCTADECANE	308.20	0.97	65
61	135	N-OCTADECANE	308.20	0.87	65
80	135	N-OCTADECANE	308.20	0.88	65
32	129	PALMITANITRILE	313.20	1.04	59
72	129	PALMITANITRILE	313.20	1.13	59
20	129	PALMITANITRILE	313.20	1.95	59
6	129	PALMITANITRILE	313.20	0.52	59
82	129	PALMITANITRILE	313.20	1.38	59
4	129	PALMITANITRILE	313.20	0.39	59
36	129	PALMITANITRILE	313.20	1.15	59
2	129	PALMITANITRILE	313.20	0.71	59
48	129	PALMITANITRILE	313.20	1.04	59
73	129	PALMITANITRILE	313.20	1.19	59
61	129	PALMITANITRILE	313.20	1.32	59
80	129	PALMITANITRILE	313.20	1.42	59
66	129	PALMITANITRILE	313.20	0.67	59
98	129	PALMITANITRILE	313.20	1.51	59
18	129	PALMITANITRILE	313.20	0.67	59
95	129	PALMITANITRILE	313.20	1.27	59
50	129	PALMITANITRILE	313.20	1.12	59
85	129	PALMITANITRILE	313.20	1.45	59
28	129	PALMITANITRILE	313.20	0.72	59
16	129	PALMITANITRILE	313.20	1.66	59
17	129	PALMITANITRILE	313.20	0.83	59
83	129	PALMITANITRILE	313.20	1.44	59
6	130	1-HEXADECENE	313.20	1.16	59
61	130	1-HEXADECENE	313.20	0.89	59

SLT	SLV		TEMP	GAMMA	REF
ID	ID	SOLVENT		INF.	
2	130	1-HEXADECENE	313.20	0.78	59
66	130	1-HEXADECENE	313.20	0.93	59
16	130	1-HEXADECENE	313.20	8.09	59
72	130	1-HEXADECENE	313.20	0.80	59
18	130	1-HEXADECENE	313.20	1.01	59
73	130	1-HEXADECENE	313.20	0.90	59
28	130	1-HEXADECENE	313.20	1.01	59
80	130	1-HEXADECENE	313.20	0.91	59
36	130	1-HEXADECENE	313.20	2.11	59
82	130	1-HEXADECENE	313.20	0.90	59
50	130	1-HEXADECENE	313.20	0.88	59
83	130	1-HEXADECENE	313.20	0.96	59
17	130	1-HEXADECENE	313.20	1.13	59
85	130	1-HEXADECENE	313.20	0.95	59
32	130	1-HEXADECENE	313.20	2.41	59
95	130	1-HEXADECENE	313.20	0.92	59
4	130	1-HEXADECENE	313.20	0.87	59
48	130	1-HEXADECENE	313.20	0.83	59
20	130	1-HEXADECENE	313.20	8.81	59
98	130	1-HEXADECENE	313.20	0.94	59
61	131	N-HEXADECYL CHLORIDE	313.20	0.97	59
85	131	N-HEXADECYL CHLORIDE	313.20	1.03	59
36	131	N-HEXADECYL CHLORIDE	313.20	1.49	59
48	131	N-HEXADECYL CHLORIDE	313.20	0.83	59
2	131	N-HEXADECYL CHLORIDE	313.20	0.75	59
50	131	N-HEXADECYL CHLORIDE	313.20	0.91	59
6	131	N-HEXADECYL CHLORIDE	313.20	0.89	59
66	131	N-HEXADECYL CHLORIDE	313.20	0.74	59
17	131	N-HEXADECYL CHLORIDE	313.20	0.80	59
72	131	N-HEXADECYL CHLORIDE	313.20	0.83	59
20	131	N-HEXADECYL CHLORIDE	313.20	4.10	59
73	131	N-HEXADECYL CHLORIDE	313.20	0.93	59
32	131	N-HEXADECYL CHLORIDE	313.20	1.60	59
80	131	N-HEXADECYL CHLORIDE	313.20	0.99	59
4	131	N-HEXADECYL CHLORIDE	313.20	0.69	59
82	131	N-HEXADECYL CHLORIDE	313.20	0.98	59
18	131	N-HEXADECYL CHLORIDE	313.20	0.81	59
83	131	N-HEXADECYL CHLORIDE	313.20	1.04	59
95	131	N-HEXADECYL CHLORIDE	313.20	0.95	59
28	131	N-HEXADECYL CHLORIDE	313.20	0.82	59
13	131	N-HEXADECYL CHLORIDE	313.20	4.16	59
98	131	N-HEXADECYL CHLORIDE	313.20	1.00	59
85	132	N-HEXADECYL BROMIDE	313.20	1.13	59
36	132	N-HEXADECYL BROMIDE	313.20	1.68	59
83	132	N-HEXADECYL BROMIDE	313.20	1.13	59
48	132	N-HEXADECYL BROMIDE	313.20	0.87	59
4	132	N-HEXADECYL BROMIDE	313.20	0.71	59
50	132	N-HEXADECYL BROMIDE	313.20	0.91	59

SLT	SLV			TEMP	GAMMA	
ID	ID	SOLVENT			INF.	REF
16	132	N-HEXADECYL BROMIDE		313.20	3.56	59
61	132	N-HEXADECYL BROMIDE		313.20	1.06	59
18	132	N-HEXADECYL BROMIDE		313.20	0.85	59
66	132	N-HEXADECYL BROMIDE		313.20	0.77	59
20	132	N-HEXADECYL BROMIDE		313.20	4.25	59
72	132	N-HEXADECYL BROMIDE		313.20	0.86	59
32	132	N-HEXADECYL BROMIDE		313.20	1.82	59
73	132	N-HEXADECYL BROMIDE		313.20	1.01	59
6	132	N-HEXADECYL BROMIDE		313.20	0.90	59
80	132	N-HEXADECYL BROMIDE		313.20	1.08	59
95	132	N-HEXADECYL BROMIDE		313.20	1.01	59
82	132	N-HEXADECYL BROMIDE		313.20	1.06	59
2	132	N-HEXADECYL BROMIDE		313.20	0.76	59
28	132	N-HEXADECYL BROMIDE		313.20	0.88	59
17	132	N-HEXADECYL BROMIDE		313.20	0.98	59
98	132	N-HEXADECYL BROMIDE		313.20	1.13	59
8	133	N-HEXADECANE		313.20	45.00	58
32	133	N-HEXADECANE		313.20	2.80	59
85	133	N-HEXADECANE		313.20	0.88	58
82	133	N-HEXADECANE		313.20	0.88	58
117	133	N-HEXADECANE		313.20	0.95	61
31	133	N-HEXADECANE		313.20	19.50	58
6	133	N-HEXADECANE		313.20	1.41	58
85	133	N-HEXADECANE		313.20	0.92	58
2	133	N-HEXADECANE		313.20	0.82	58
32	133	N-HEXADECANE		313.20	3.10	58
109	133	N-HEXADECANE		313.20	0.93	61
16	133	N-HEXADECANE		313.20	9.99	58
98	133	N-HEXADECANE		313.20	0.91	61
36	133	N-HEXADECANE		313.20	2.50	58
19	133	N-HEXADECANE		313.20	30.50	58
36	133	N-HEXADECANE		313.20	2.44	59
21	133	N-HEXADECANE		313.20	5.10	58
42	133	N-HEXADECANE		313.20	0.85	61
22	133	N-HEXADECANE		313.20	3.20	58
48	133	N-HEXADECANE		313.20	0.83	59
28	133	N-HEXADECANE		313.20	1.12	58
50	133	N-HEXADECANE		313.20	0.86	59
80	133	N-HEXADECANE		313.20	0.89	61
59	133	N-HEXADECANE		313.20	1.80	58
4	133	N-HEXADECANE		313.20	1.02	58
61	133	N-HEXADECANE		313.20	0.87	61
98	133	N-HEXADECANE		313.20	0.93	59
75	133	N-HEXADECANE		313.20	0.71	58
61	133	N-HEXADECANE		313.20	0.86	58
95	133	N-HEXADECANE		313.20	0.93	58
66	133	N-HEXADECANE		313.20	1.01	59
30	133	N-HEXADECANE		313.20	0.82	61

SLT	SLV		TEMP	GAMMA	REF
ID	ID	SOLVENT		INF.	
83	133	N-HEXADECANE	313.20	0.90	58
18	133	N-HEXADECANE	313.20	1.16	58
72	133	N-HEXADECANE	313.20	0.79	59
23	133	N-HEXADECANE	313.20	3.10	58
20	133	N-HEXADECANE	313.20	10.50	58
17	133	N-HEXADECANE	313.20	1.25	58
73	133	N-HEXADECANE	313.20	0.91	58
2	80	N-HEXANE	315.00	1.20	1
70	80	N-HEXANE	315.10	5.30	1
32	80	N-HEXANE	315.30	3.97	1
24	80	N-HEXANE	315.30	11.50	1
40	80	N-HEXANE	315.30	1.40	1
72	80	N-HEXANE	315.30	1.09	1
31	80	N-HEXANE	315.30	26.10	1
43	80	N-HEXANE	315.30	22.50	1
18	80	N-HEXANE	315.30	1.54	1
4	80	N-HEXANE	315.30	1.53	1
39	80	N-HEXANE	315.30	1.50	1
44	80	N-HEXANE	316.00	4.83	1
14	80	N-HEXANE	316.00	2.73	1
36	80	N-HEXANE	316.00	2.95	1
16	80	N-HEXANE	316.00	15.20	1
91	80	N-HEXANE	322.80	1.46	1
34	80	N-HEXANE	322.80	1.59	1
19	80	N-HEXANE	322.80	23.00	1
87	80	N-HEXANE	322.90	1.10	1
11	80	N-HEXANE	322.90	16.80	1
9	80	N-HEXANE	322.90	23.90	1
20	80	N-HEXANE	322.90	13.60	1
17	80	N-HEXANE	322.90	1.87	1
80	87	TRIETHYLAMINE	323.50	1.06	1
14	87	TRIETHYLAMINE	323.50	1.44	1
86	87	TRIETHYLAMINE	323.50	1.28	1
98	134	N-HEXADECANOL	326.30	1.76	64
99	134	N-HEXADECANOL	326.30	1.75	64
71	134	N-HEXADECANOL	326.30	1.58	64
50	134	N-HEXADECANOL	326.30	1.43	64
100	134	N-HEXADECANOL	326.30	1.85	64
48	134	N-HEXADECANOL	326.30	1.31	64
72	134	N-HEXADECANOL	326.30	1.29	64
15	134	N-HEXADECANOL	326.30	1.36	64
73	134	N-HEXADECANOL	326.30	1.53	64
81	134	N-HEXADECANOL	326.30	1.55	64
74	134	N-HEXADECANOL	326.30	1.42	64
82	134	N-HEXADECANOL	326.30	1.59	64
75	134	N-HEXADECANOL	326.30	1.34	64
89	134	N-HEXADECANOL	326.30	1.18	64
47	134	N-HEXADECANOL	326.30	1.17	64

SLT	SLV			GAMMA	
ID	ID	SOLVENT	TEMP	INF.	REF
28	134	N-HEXADECANOL	326.30	1.34	64
91	134	N-HEXADECANOL	326.30	1.23	64
2	134	N-HEXADECANOL	326.30	1.11	64
80	134	N-HEXADECANOL	326.30	1.65	64
95	134	N-HEXADECANOL	326.30	1.63	64
85	134	N-HEXADECANOL	326.30	1.71	64
5	134	N-HEXADECANOL	326.30	0.90	64
81	134	N-HEXADECANOL	326.30	1.62	64
66	134	N-HEXADECANOL	326.30	1.21	64
38	134	N-HEXADECANOL	326.30	1.49	64
3	134	N-HEXADECANOL	326.30	1.10	64
83	134	N-HEXADECANOL	326.30	1.72	64
6	134	N-HEXADECANOL	326.30	1.13	64
7	134	N-HEXADECANOL	326.30	1.47	64
14	134	N-HEXADECANOL	326.30	1.67	64
4	134	N-HEXADECANOL	326.30	0.84	64
10	134	N-HEXADECANOL	326.30	1.22	64
39	134	N-HEXADECANOL	326.30	1.43	64
69	136	N-EICOSANE	326.30	0.73	64
95	136	N-EICOSANE	326.30	0.92	64
50	136	N-EICOSANE	326.30	0.85	64
14	136	N-EICOSANE	326.30	1.59	64
10	136	N-EICOSANE	326.30	1.01	64
4	136	N-EICOSANE	326.30	0.89	64
28	136	N-EICOSANE	326.30	1.02	64
48	136	N-EICOSANE	326.30	0.79	64
91	136	N-EICOSANE	326.30	0.89	64
6	136	N-EICOSANE	326.30	1.15	64
47	136	N-EICOSANE	326.30	0.69	64
72	136	N-EICOSANE	326.30	0.74	64
75	136	N-EICOSANE	326.30	0.77	64
73	136	N-EICOSANE	326.30	0.88	64
85	136	N-EICOSANE	326.30	0.92	64
66	136	N-EICOSANE	326.30	0.90	64
80	136	N-EICOSANE	326.30	0.89	64
74	136	N-EICOSANE	326.30	0.83	64
81	136	N-EICOSANE	326.30	0.88	64
3	136	N-EICOSANE	326.30	0.81	64
62	136	N-EICOSANE	326.30	0.88	64
71	136	N-EICOSANE	326.30	0.90	64
38	136	N-EICOSANE	326.30	1.06	64
5	136	N-EICOSANE	326.30	0.98	64
61	136	N-EICOSANE	326.30	0.85	64
15	136	N-EICOSANE	326.30	1.17	64
83	136	N-EICOSANE	326.30	0.92	64
100	136	N-EICOSANE	326.30	0.97	64
39	136	N-EICOSANE	326.30	1.03	64
98	136	N-EICOSANE	326.30	0.92	64

SLT	SLV		TEMP	GAMMA	REF
ID	ID	SOLVENT		INF.	
99	136	N-EICOSANE	326.30	0.92	64
2	136	N-EICOSANE	326.30	0.78	64
7	136	N-EICOSANE	326.30	1.48	64
28	142	N-SQUALANE	326.30	0.70	64
98	142	N-SQUALANE	326.30	0.70	64
7	142	N-SQUALANE	326.30	1.06	64
69	142	N-SQUALANE	326.30	0.52	64
6	142	N-SQUALANE	326.30	0.79	64
71	142	N-SQUALANE	326.30	0.67	64
2	142	N-SQUALANE	326.30	0.56	64
75	142	N-SQUALANE	326.30	0.55	64
85	142	N-SQUALANE	326.30	0.68	64
80	142	N-SQUALANE	326.30	0.67	64
84	142	N-SQUALANE	326.30	0.67	64
66	142	N-SQUALANE	326.30	0.65	64
74	142	N-SQUALANE	326.30	0.61	64
91	142	N-SQUALANE	326.30	0.66	64
39	142	N-SQUALANE	326.30	0.73	64
81	142	N-SQUALANE	326.30	0.64	64
61	142	N-SQUALANE	326.30	0.63	64
50	142	N-SQUALANE	326.30	0.62	64
15	142	N-SQUALANE	326.30	0.82	64
5	142	N-SQUALANE	326.30	0.71	64
47	142	N-SQUALANE	326.30	0.49	64
48	142	N-SQUALANE	326.30	0.57	64
10	142	N-SQUALANE	326.30	0.71	64
99	142	N-SQUALANE	326.30	0.69	64
84	142	N-SQUALANE	326.30	0.73	64
72	142	N-SQUALANE	326.30	0.53	64
95	142	N-SQUALANE	326.30	0.69	64
62	142	N-SQUALANE	326.30	0.64	64
14	142	N-SQUALANE	326.30	1.06	64
4	142	N-SQUALANE	326.30	0.65	64
73	142	N-SQUALANE	326.30	0.66	64
38	142	N-SQUALANE	326.30	0.75	64
100	142	N-SQUALANE	326.30	0.72	64
83	142	N-SQUALANE	326.30	0.67	64
3	142	N-SQUALANE	326.30	0.61	64
17	80	N-HEXANE	329.10	1.83	1
87	80	N-HEXANE	330.10	1.83	1
44	80	N-HEXANE	330.10	4.22	1
66	98	N-HEPTANE	331.00	1.37	2
31	80	N-HEXANE	331.00	10.00	1
43	80	N-HEXANE	331.00	15.10	1
4	80	N-HEXANE	331.00	1.00	1
40	80	N-HEXANE	331.00	1.35	1
16	80	N-HEXANE	331.00	12.30	1
36	80	N-HEXANE	331.00	2.60	1

SLT	SLV		TEMP	GAMMA	REF
ID	ID	SOLVENT		INF.	
18	80	N-HEXANE	332.00	1.37	1
39	80	N-HEXANE	332.00	1.43	1
32	80	N-HEXANE	332.00	3.60	1
72	80	N-HEXANE	332.00	1.07	1
70	80	N-HEXANE	332.00	4.70	1
14	80	N-HEXANE	332.00	2.45	1
2	80	N-HEXANE	332.00	1.19	1
24	80	N-HEXANE	332.00	9.60	1
20	80	N-HEXANE	332.20	10.70	1
11	80	N-HEXANE	332.30	13.70	1
9	80	N-HEXANE	332.30	19.90	1
80	133	N-HEXADECANE	333.15	0.88	58
42	126	N-DECANE	333.20	0.99	58
75	126	N-DECANE	333.20	0.93	58
82	126	N-DECANE	333.20	0.98	58
72	126	N-DECANE	333.20	0.94	58
85	126	N-DECANE	333.20	0.99	58
62	126	N-DECANE	333.20	0.98	58
98	126	N-DECANE	333.20	0.98	58
61	126	N-DECANE	333.20	0.97	58
83	126	N-DECANE	333.20	0.99	58
80	126	N-DECANE	333.20	0.97	58
94	126	N-DECANE	333.20	0.92	58
81	126	N-DECANE	333.20	0.98	58
98	133	N-HEXADECANE	333.20	0.89	58
72	133	N-HEXADECANE	333.20	0.75	58
47	133	N-HEXADECANE	333.20	0.73	58
66	133	N-HEXADECANE	333.20	0.90	58
83	133	N-HEXADECANE	333.20	0.91	58
94	133	N-HEXADECANE	333.20	0.79	58
75	133	N-HEXADECANE	333.20	0.77	58
61	133	N-HEXADECANE	333.20	0.87	58
48	134	N-HEXADECANOL	333.20	1.12	59
72	134	N-HEXADECANOL	333.20	1.15	59
18	134	N-HEXADECANOL	333.20	1.06	59
98	134	N-HEXADECANOL	333.20	1.59	59
73	134	N-HEXADECANOL	333.20	1.35	59
6	134	N-HEXADECANOL	333.20	0.97	59
80	134	N-HEXADECANOL	333.20	1.47	59
82	134	N-HEXADECANOL	333.20	1.43	59
66	134	N-HEXADECANOL	333.20	1.07	59
20	134	N-HEXADECANOL	333.20	3.76	59
83	134	N-HEXADECANOL	333.20	1.48	59
36	134	N-HEXADECANOL	333.20	1.50	59
17	134	N-HEXADECANOL	333.20	1.22	59
50	134	N-HEXADECANOL	333.20	1.18	59
85	134	N-HEXADECANOL	333.20	1.52	59
61	134	N-HEXADECANOL	333.20	1.29	59

SLT	SLV	SOLVENT	TEMP	GAMMA INF.	REF
95	134	N-HEXADECANOL	333.20	1.47	59
28	134	N-HEXADECANOL	333.20	1.14	59
4	134	N-HEXADECANOL	333.20	0.76	59
32	134	N-HEXADECANOL	333.20	1.49	59
31	91	TOLUENE	338.20	6.24	17
14	91	TOLUENE	338.20	1.00	17
14	80	N-HEXANE	339.40	2.32	1
35	80	N-HEXANE	339.40	2.39	1
16	80	N-HEXANE	339.40	10.00	1
4	80	N-HEXANE	340.10	1.39	1
40	80	N-HEXANE	340.10	1.27	1
31	80	N-HEXANE	340.10	13.70	1
34	80	N-HEXANE	340.20	1.51	1
2	80	N-HEXANE	340.30	1.16	1
39	80	N-HEXANE	340.30	1.40	1
72	80	N-HEXANE	340.30	1.06	1
43	80	N-HEXANE	340.30	12.20	1
24	80	N-HEXANE	340.30	8.50	1
18	80	N-HEXANE	340.30	1.26	1
32	80	N-HEXANE	340.30	3.40	1
44	80	N-HEXANE	340.60	4.04	1
9	80	N-HEXANE	340.90	17.80	1
11	80	N-HEXANE	340.90	12.40	1
20	80	N-HEXANE	340.90	10.00	1
24	91	TOLUENE	342.70	1.85	1
32	91	TOLUENE	342.70	1.39	1
36	91	TOLUENE	342.70	1.21	1
16	91	TOLUENE	342.70	2.35	1
19	91	TOLUENE	342.90	6.95	1
117	133	N-HEXADECANE	343.20	0.94	61
30	133	N-HEXADECANE	343.20	0.81	61
98	133	N-HEXADECANE	343.20	0.90	61
126	133	N-HEXADECANE	343.20	0.96	61
109	133	N-HEXADECANE	343.20	0.92	61
42	133	N-HEXADECANE	343.20	0.84	61
61	133	N-HEXADECANE	343.20	0.86	61
80	133	N-HEXADECANE	343.20	0.88	61
72	134	N-HEXADECANOL	347.30	1.18	64
95	134	N-HEXADECANOL	347.30	1.51	64
7	134	N-HEXADECANOL	347.30	1.26	64
81	134	N-HEXADECANOL	347.30	1.49	64
4	134	N-HEXADECANOL	347.30	0.80	64
38	134	N-HEXADECANOL	347.30	1.32	64
75	134	N-HEXADECANOL	347.30	1.25	64
83	134	N-HEXADECANOL	347.30	1.58	64
48	134	N-HEXADECANOL	347.30	1.22	64
69	134	N-HEXADECANOL	347.30	1.08	64
6	134	N-HEXADECANOL	347.30	0.99	64

SLT	SLV		TEMP	GAMMA	REF
ID	ID	SOLVENT		INF.	
39	134	N-HEXADECANOL	347.30	1.28	64
98	134	N-HEXADECANOL	347.30	1.64	64
3	134	N-HEXADECANOL	347.30	1.03	64
62	134	N-HEXADECANOL	347.30	1.48	64
15	134	N-HEXADECANOL	347.30	1.18	64
99	134	N-HEXADECANOL	347.30	1.62	64
91	134	N-HEXADECANOL	347.30	1.13	64
74	134	N-HEXADECANOL	347.30	1.32	64
14	134	N-HEXADECANOL	347.30	1.41	64
61	134	N-HEXADECANOL	347.30	1.42	64
10	134	N-HEXADECANOL	347.30	1.07	64
73	134	N-HEXADECANOL	347.30	1.41	64
85	134	N-HEXADECANOL	347.30	1.59	64
50	134	N-HEXADECANOL	347.30	1.31	64
66	134	N-HEXADECANOL	347.30	1.07	64
100	134	N-HEXADECANOL	347.30	1.70	64
2	134	N-HEXADECANOL	347.30	1.03	64
71	134	N-HEXADECANOL	347.30	1.44	64
47	134	N-HEXADECANOL	347.30	1.09	64
5	134	N-HEXADECANOL	347.30	0.85	64
80	134	N-HEXADECANOL	347.30	1.53	64
28	134	N-HEXADECANOL	347.30	1.19	64
48	136	N-EICOSANE	347.30	0.77	64
4	136	N-EICOSANE	347.30	0.83	64
7	136	N-EICOSANE	347.30	1.29	64
72	136	N-EICOSANE	347.30	0.73	64
66	136	N-EICOSANE	347.30	0.85	64
50	136	N-EICOSANE	347.30	0.81	64
6	136	N-EICOSANE	347.30	1.01	64
38	136	N-EICOSANE	347.30	0.59	64
85	136	N-EICOSANE	347.30	0.89	64
61	136	N-EICOSANE	347.30	0.83	64
69	136	N-EICOSANE	347.30	0.71	64
100	136	N-EICOSANE	347.30	0.95	64
71	136	N-EICOSANE	347.30	0.87	64
99	136	N-EICOSANE	347.30	0.91	64
83	136	N-EICOSANE	347.30	0.89	64
98	136	N-EICOSANE	347.30	0.91	64
81	136	N-EICOSANE	347.30	0.86	64
10	136	N-EICOSANE	347.30	0.92	64
80	136	N-EICOSANE	347.30	0.88	64
47	136	N-EICOSANE	347.30	0.68	64
75	136	N-EICOSANE	347.30	0.75	64
28	136	N-EICOSANE	347.30	0.94	64
2	136	N-EICOSANE	347.30	0.73	64
14	136	N-EICOSANE	347.30	1.39	64
74	136	N-EICOSANE	347.30	0.82	64
95	136	N-EICOSANE	347.30	0.90	64

SLT	SLV		TEMP	GAMMA	REF
ID	ID	SOLVENT		INF	
5	136	N-FICOSANE	347.30	0.90	64
39	136	N-EICOSANE	347.30	0.98	64
3	136	N-EICOSANE	347.30	0.78	64
62	136	N-EICOSANE	347.30	0.84	64
15	136	N-EICOSANE	347.30	1.06	64
91	136	N-EICOSANE	347.30	0.86	64
73	136	N-EICOSANE	347.30	0.87	64
74	142	N-SQUALANE	347.30	0.62	64
95	142	N-SQUALANE	347.30	0.70	64
4	142	N-SQUALANE	347.30	0.62	64
3	142	N-SQUALANE	347.30	0.59	64
61	142	N-SQUALANE	347.30	0.62	64
38	142	N-SQUALANE	347.30	0.72	64
15	142	N-SQUALANE	347.30	0.77	64
72	142	N-SQUALANE	347.30	0.53	64
69	142	N-SQUALANE	347.30	0.52	64
100	142	N-SQUALANE	347.30	0.72	64
14	142	N-SQUALANE	347.30	0.97	64
99	142	N-SQUALANE	347.30	0.69	64
10	142	N-SQUALANE	347.30	0.67	64
28	142	N-SQUALANE	347.30	0.67	64
80	142	N-SQUALANE	347.30	0.66	64
98	142	N-SQUALANE	347.30	0.70	64
7	142	N-SQUALANE	347.30	0.95	64
83	142	N-SQUALANE	347.30	0.66	64
48	142	N-SQUALANE	347.30	0.57	64
66	142	N-SQUALANE	347.30	0.63	64
84	142	N-SQUALANE	347.30	0.73	64
84	142	N-SQUALANE	347.30	0.66	64
6	142	N-SQUALANE	347.30	0.73	64
91	142	N-SQUALANE	347.30	0.66	64
75	142	N-SQUALANE	347.30	0.56	64
81	142	N-SQUALANE	347.30	0.64	64
5	142	N-SQUALANE	347.30	0.68	64
73	142	N-SQUALANE	347.30	0.66	64
2	142	N-SQUALANE	347.30	0.54	64
62	142	N-SQUALANE	347.30	0.62	64
71	142	N-SQUALANE	347.30	0.66	64
85	142	N-SQUALANE	347.30	0.67	64
47	142	N-SQUALANE	347.30	0.49	64
39	142	N-SQUALANE	347.30	0.71	64
50	142	N-SQUALANE	347.30	0.61	64
66	87	TRIETHYLAMINE	348.70	1.22	1
80	87	TRIETHYLAMINE	348.70	1.06	1
9	87	TRIETHYLAMINE	348.70	6.70	1
11	87	TRIETHYLAMINE	348.70	5.50	1
18	87	TRIETHYLAMINE	348.70	1.02	1
14	87	TRIETHYLAMINE	348.70	1.40	1

SLT	SLV	SOLVENT	TEMP	GAMMA	REF
ID	ID			INF.	
66	98	N-HEPTANE	350.60	1.33	1
50	140	SQUALENE	353.15	0.63	63
36	140	SQUALENE	353.15	1.04	63
66	142	N-SQUALANE	353.15	0.59	63
50	142	N-SQUALANE	353.15	0.61	58
16	135	N-OCTADECANE	353.20	5.90	63
11	135	N-OCTADECANE	353.20	9.70	63
57	135	N-OCTADECANE	353.20	1.69	63
21	135	N-OCTADECANE	353.20	2.96	63
25	135	N-OCTADECANE	353.20	8.20	63
36	135	N-OCTADECANE	353.20	1.86	63
80	135	N-OCTADECANE	353.20	0.84	63
1	135	N-OCTADECANE	353.20	0.65	63
66	135	N-OCTADECANE	353.20	0.83	63
20	135	N-OCTADECANE	353.20	6.50	63
73	135	N-OCTADECANE	353.20	0.84	63
32	135	N-OCTADECANE	353.20	2.20	63
14	135	N-OCTADECANE	353.20	1.33	63
80	136	N-EICOSANE	353.20	0.87	69
83	136	N-EICOSANE	353.20	0.90	69
126	136	N-EICOSANE	353.20	0.97	69
61	136	N-EICOSANE	353.20	0.83	69
85	136	N-EICOSANE	353.20	0.89	69
82	136	N-EICOSANE	353.20	0.86	69
109	136	N-EICOSANE	353.20	0.92	69
81	136	N-EICOSANE	353.20	0.86	69
62	136	N-EICOSANE	353.20	0.86	69
98	136	N-EICOSANE	353.20	0.90	69
108	136	N-EICOSANE	353.20	0.97	69
47	138	N-TETRACOSANE	353.20	0.57	58
75	138	N-TETRACOSANE	353.20	0.61	58
98	138	N-TETRACOSANE	353.20	0.73	58
62	138	N-TETRACOSANE	353.20	0.73	58
80	138	N-TETRACOSANE	353.20	0.73	58
66	138	N-TETRACOSANE	353.20	0.63	58
83	138	N-TETRACOSANE	353.20	0.76	58
103	138	N-TETRACOSANE	353.20	0.64	58
91	138	N-TETRACOSANE	353.20	0.64	58
109	138	N-TETRACOSANE	353.20	0.74	58
61	138	N-TETRACOSANE	353.20	0.73	58
72	138	N-TETRACOSANE	353.20	0.58	58
94	138	N-TETRACOSANE	353.20	0.59	58
57	140	SQUALENE	353.20	0.89	63
11	140	SQUALENE	353.20	3.82	63
16	140	SQUALENE	353.20	2.48	63
14	140	SQUALENE	353.20	0.66	63
32	140	SQUALENE	353.20	1.14	63
21	140	SQUALENE	353.20	1.42	63

SLT	SLV		TEMP	GAMMA	REF
ID	ID	SOLVENT		INF.	
1	140	SQUALENE	353.20	0.40	63
20	140	SQUALENE	353.20	2.78	63
25	140	SQUALENE	353.20	3.03	63
80	140	SQUALENE	353.20	0.69	63
66	140	SQUALENE	353.20	0.50	63
73	140	SQUALENE	353.20	0.63	63
32	142	N-SQUALANE	353.20	1.50	63
72	142	N-SQUALANE	353.20	0.51	58
83	142	N-SQUALANE	353.20	0.69	58
20	142	N-SQUALANE	353.20	4.40	63
98	142	N-SQUALANE	353.20	0.67	58
80	142	N-SQUALANE	353.20	0.61	63
61	142	N-SQUALANE	353.20	0.66	58
21	142	N-SQUALANE	353.20	1.93	63
75	142	N-SQUALANE	353.20	0.55	58
36	142	N-SQUALANE	353.20	1.27	63
1	142	N-SQUALANE	353.20	0.45	63
25	142	N-SQUALANE	353.20	5.40	63
80	142	N-SQUALANE	353.20	0.66	58
57	142	N-SQUALANE	353.20	1.17	63
14	142	N-SQUALANE	353.20	0.89	63
109	142	N-SQUALANE	353.20	0.69	58
11	142	N-SQUALANE	353.20	6.40	63
62	142	N-SQUALANE	353.20	0.67	58
73	142	N-SQUALANE	353.20	0.61	63
66	142	N-SQUALANE	353.20	0.58	58
47	142	N-SQUALANE	353.20	0.51	58
94	142	N-SQUALANE	353.20	0.54	58
16	142	N-SQUALANE	353.20	3.85	63
103	142	N-SQUALANE	353.20	0.61	58
91	142	N-SQUALANE	353.20	0.60	58
72	144	N-PENTATRIACONTANE	353.20	0.47	58
103	144	N-PENTATRIACONTANE	353.20	0.52	58
98	144	N-PENTATRIACONTANE	353.20	0.63	58
75	144	N-PENTATRIACONTANE	353.20	0.50	58
80	144	N-PENTATRIACONTANE	353.20	0.61	58
109	144	N-PENTATRIACONTANE	353.20	0.65	58
61	144	N-PENTATRIACONTANE	353.20	0.62	58
62	144	N-PENTATRIACONTANE	353.20	0.62	58
47	144	N-PENTATRIACONTANE	353.20	0.46	58
94	144	N-PENTATRIACONTANE	353.20	0.50	58
91	144	N-PENTATRIACONTANE	353.20	0.52	58
66	144	N-PENTATRIACONTANE	353.20	0.51	58
83	144	N-PENTATRIACONTANE	353.20	0.64	58
80	87	TRIETHYLAMINE	359.30	1.06	1
66	87	TRIETHYLAMINE	359.30	1.08	1
14	87	TRIETHYLAMINE	359.30	1.35	1
19	91	TOLUENE	362.70	6.00	1

SLT	SLV		TEMP	GAMMA	REF
ID	ID	SOLVENT		INF	
36	91	TOLUENE	362.70	1.20	1
32	91	TOLUENE	362.70	1.35	1
16	91	TOLUENE	362.70	2.23	1
24	91	TOLUENE	362.70	1.73	1
8	91	TOLUENE	362.70	8.10	1
42	133	N-HEXADECANE	363.20	0.83	61
61	133	N-HEXADECANE	363.20	0.85	61
117	133	N-HEXADECANE	363.20	0.94	61
109	133	N-HEXADECANE	363.20	0.92	61
30	133	N-HEXADECANE	363.20	0.80	61
80	133	N-HEXADECANE	363.20	0.88	61
98	133	N-HEXADECANE	363.20	0.90	61
126	133	N-HEXADECANE	363.20	0.95	61
66	98	N-HEPTANE	366.20	1.27	1
62	134	N-HEXADECANOL	367.10	1.40	64
80	134	N-HEXADECANOL	367.10	1.48	64
72	134	N-HEXADECANOL	367.10	1.14	64
61	134	N-HEXADECANOL	367.10	1.36	64
66	134	N-HEXADECANOL	367.10	1.01	64
3	134	N-HEXADECANOL	367.10	1.00	64
69	134	N-HEXADECANOL	367.10	1.04	64
5	134	N-HEXADECANOL	367.10	0.83	64
98	134	N-HEXADECANOL	367.10	1.60	64
7	134	N-HEXADECANOL	367.10	1.14	64
99	134	N-HEXADECANOL	367.10	1.57	64
14	134	N-HEXADECANOL	367.10	1.26	64
100	134	N-HEXADECANOL	367.10	1.64	64
28	134	N-HEXADECANOL	367.10	1.10	64
91	134	N-HEXADECANOL	367.10	1.08	64
39	134	N-HEXADECANOL	367.10	1.20	64
85	134	N-HEXADECANOL	367.10	1.51	64
48	134	N-HEXADECANOL	367.10	1.16	64
83	134	N-HEXADECANOL	367.10	1.51	64
95	134	N-HEXADECANOL	367.10	1.46	64
71	134	N-HEXADECANOL	367.10	1.36	64
6	134	N-HEXADECANOL	367.10	0.90	64
81	134	N-HEXADECANOL	367.10	1.43	64
15	134	N-HEXADECANOL	367.10	1.09	64
75	134	N-HEXADECANOL	367.10	1.20	64
47	134	N-HEXADECANOL	367.10	1.05	64
74	134	N-HEXADECANOL	367.10	1.27	64
4	134	N-HEXADECANOL	367.10	0.80	64
73	134	N-HEXADECANOL	367.10	1.35	64
38	134	N-HEXADECANOL	367.10	1.21	64
10	134	N-HEXADECANOL	367.10	1.00	64
50	134	N-HEXADECANOL	367.10	1.24	64
2	134	N-HEXADECANOL	367.10	1.00	64
72	136	N-EICOSANE	367.10	0.72	64

SLT	SLV		TEMP	GAMMA	REF
ID	ID	SOLVENT		INF.	
28	136	N-EICOSANE	367.10	0.90	64
85	136	N-EICOSANE	367.10	0.88	64
74	136	N-EICOSANE	367.10	0.81	64
15	136	N-EICOSANE	367.10	0.98	64
71	136	N-EICOSANE	367.10	0.85	64
14	136	N-EICOSANE	367.10	1.26	64
80	136	N-EICOSANE	367.10	0.87	64
10	136	N-EICOSANE	367.10	0.88	64
62	136	N-EICOSANE	367.10	0.82	64
7	136	N-EICOSANE	367.10	1.18	64
61	136	N-EICOSANE	367.10	0.82	64
6	136	N-EICOSANE	367.10	0.92	64
48	136	N-EICOSANE	367.10	0.76	64
91	136	N-EICOSANE	367.10	0.85	64
39	136	N-EICOSANE	367.10	0.94	64
5	136	N-EICOSANE	367.10	0.86	64
38	136	N-EICOSANE	367.10	0.94	64
4	136	N-EICOSANE	367.10	0.80	64
75	136	N-EICOSANE	367.10	0.75	64
95	136	N-EICOSANE	367.10	0.90	64
66	136	N-EICOSANE	367.10	0.82	64
3	136	N-EICOSANE	367.10	0.77	64
50	136	N-EICOSANE	367.10	0.80	64
2	136	N-EICOSANE	367.10	0.72	64
83	136	N-EICOSANE	367.10	0.87	64
98	136	N-EICOSANE	367.10	0.92	64
69	136	N-EICOSANE	367.10	0.71	64
99	136	N-EICOSANE	367.10	0.90	64
47	136	N-EICOSANE	367.10	0.67	64
81	136	N-EICOSANE	367.10	0.85	64
73	136	N-EICOSANE	367.10	0.86	64
100	136	N-EICOSANE	367.10	0.94	64
4	142	N-SQUALANE	367.10	0.62	64
85	142	N-SQUALANE	367.10	0.68	64
69	142	N-SQUALANE	367.10	0.54	64
84	142	N-SQUALANE	367.10	0.68	64
100	142	N-SQUALANE	367.10	0.74	64
62	142	N-SQUALANE	367.10	0.63	64
80	142	N-SQUALANE	367.10	0.68	64
72	142	N-SQUALANE	367.10	0.54	64
50	142	N-SQUALANE	367.10	0.61	64
2	142	N-SQUALANE	367.10	0.55	64
3	142	N-SQUALANE	367.10	0.60	64
47	142	N-SQUALANE	367.10	0.50	64
99	142	N-SQUALANE	367.10	0.71	64
73	142	N-SQUALANE	367.10	0.67	64
98	142	N-SQUALANE	367.10	0.72	64
28	142	N-SQUALANE	367.10	0.67	64

SLT	SLV	SOLVENT	TEMP	GAMMA	REF
ID	ID			INF.	
95	142	N-SQUALANE	367.10	0.72	64
74	142	N-SQUALANE	367.10	0.63	64
10	142	N-SQUALANE	367.10	0.66	64
14	142	N-SQUALANE	367.10	0.93	64
91	142	N-SQUALANE	367.10	0.66	64
84	142	N-SQUALANE	367.10	0.74	64
81	142	N-SQUALANE	367.10	0.65	64
48	142	N-SQUALANE	367.10	0.58	64
7	142	N-SQUALANE	367.10	0.90	64
38	142	N-SQUALANE	367.10	0.72	64
66	142	N-SQUALANE	367.10	0.63	64
15	142	N-SQUALANE	367.10	0.74	64
83	142	N-SQUALANE	367.10	0.67	64
61	142	N-SQUALANE	367.10	0.63	64
6	142	N-SQUALANE	367.10	0.70	64
5	142	N-SQUALANE	367.10	0.67	64
39	142	N-SQUALANE	367.10	0.72	64
75	142	N-SQUALANE	367.10	0.57	64
71	142	N-SQUALANE	367.10	0.66	64
31	133	N-HEXADECANE	373.15	4.32	62
8	133	N-HEXADECANE	373.15	8.59	62
59	133	N-HEXADECANE	373.20	1.41	62
33	133	N-HEXADECANE	373.20	1.49	62
19	133	N-HEXADECANE	373.20	5.71	62
43	133	N-HEXADECANE	373.20	3.77	62
23	133	N-HEXADECANE	373.20	1.71	62
83	138	N-TETRACOSANE	373.20	0.82	69
81	138	N-TETRACOSANE	373.20	0.75	69
85	138	N-TETRACOSANE	373.20	0.82	69
82	138	N-TETRACOSANE	373.20	0.77	69
62	138	N-TETRACOSANE	373.20	0.78	69
98	138	N-TETRACOSANE	373.20	0.83	69
80	138	N-TETRACOSANE	373.20	0.80	69
126	138	N-TETRACOSANE	373.20	0.89	69
108	138	N-TETRACOSANE	373.20	0.89	69
81	138	N-TETRACOSANE	373.20	0.78	69
109	138	N-TETRACOSANE	373.20	0.85	69
85	142	N-SQUALANE	373.20	0.67	58
14	91	TOLUENE	380.90	0.97	1
36	91	TOLUENE	380.90	1.16	1
8	91	TOLUENE	381.00	5.00	1
19	91	TOLUENE	381.00	4.39	1
16	91	TOLUENE	381.00	2.10	1
32	91	TOLUENE	381.00	1.33	1
19	133	N-HEXADECANE	393.15	4.37	62
31	133	N-HEXADECANE	393.20	3.24	62
8	133	N-HEXADECANE	393.20	6.39	62
23	133	N-HEXADECANE	393.20	1.60	62

SLT	SLV	SOLVENT	TEMP	GAMMA	REF
ID	ID			INF.	
43	133	N-HEXADECANE	393.20	2.90	62
59	133	N-HEXADECANE	393.20	1.29	62
33	133	N-HEXADECANE	393.20	1.39	62
8	133	N-HEXADECANE	403.15	5.62	62
19	133	N-HEXADECANE	403.15	3.80	62
31	133	N-HEXADECANE	403.20	2.90	62
33	133	N-HEXADECANE	403.20	1.35	62
43	133	N-HEXADECANE	403.20	2.60	62
23	133	N-HEXADECANE	403.20	1.56	62
59	133	N-HEXADECANE	403.20	1.25	62
8	133	N-HEXADECANE	413.15	4.89	62
19	133	N-HEXADECANE	413.15	3.29	62
33	133	N-HEXADECANE	413.20	1.31	62
43	133	N-HEXADECANE	413.20	2.30	62
31	133	N-HEXADECANE	413.20	2.58	62
59	133	N-HEXADECANE	413.20	1.21	62
23	133	N-HEXADECANE	413.20	1.51	62
43	79	N-BUTYL ACETATE	353.60	2.09	3 *
67	79	N-BUTYL ACETATE	399.30	0.53	3 *
67	79	N-BUTYL ACETATE	358.40	0.26	3 *
2	80	N-HEXANE	341.90	1.18	3 *
2	80	N-HEXANE	303.20	1.28	3 *
4	80	N-HEXANE	298.20	1.66	3 *
4	80	N-HEXANE	341.90	1.38	3 *
12	80	N-HEXANE	333.20	1.34	3 *
13	80	N-HEXANE	333.20	2.59	3 *
17	80	N-HEXANE	333.20	1.91	3 *
19	80	N-HEXANE	342.15	18.10	3 *
21	80	N-HEXANE	328.20	4.24	3 *
21	80	N-HEXANE	268.20	10.78	3 *
21	80	N-HEXANE	293.20	7.24	3 *
21	80	N-HEXANE	308.20	5.31	3 *
21	80	N-HEXANE	318.20	4.80	3 *
32	80	N-HEXANE	333.20	3.69	3 *
32	80	N-HEXANE	298.20	5.00	19 *
32	80	N-HEXANE	333.20	3.70	19 *
32	80	N-HEXANE	373.20	2.80	19 *
32	80	N-HEXANE	338.20	3.50	3 *
37	80	N-HEXANE	353.20	2.80	34 *
37	80	N-HEXANE	353.20	2.99	3 *
37	80	N-HEXANE	341.90	3.24	33 *
42	80	N-HEXANE	293.20	1.00	3 *
43	80	N-HEXANE	341.90	11.15	3 *
55	80	N-HEXANE	338.20	2.90	3 *
61	80	N-HEXANE	298.20	0.95	3 *
61	80	N-HEXANE	341.30	0.94	3 *
63	80	N-HEXANE	323.20	11.80	3 *
63	80	N-HEXANE	298.20	18.60	3 *

SLT	SLV	SOLVENT	TEMP	GAMMA	INF.	REF
64	80	N-HEXANE	298.20	14.50	3	*
65	80	N-HEXANE	338.20	1.83	3	*
66	80	N-HEXANE	348.20	1.47	26	*
66	80	N-HEXANE	353.15	1.49	3	*
66	80	N-HEXANE	341.90	1.46	3	*
66	80	N-HEXANE	298.20	1.73	3	*
66	80	N-HEXANE	298.20	1.66	26	*
68	80	N-HEXANE	340.20	13.80	3	*
72	80	N-HEXANE	341.90	1.06	3	*
73	80	N-HEXANE	333.20	1.03	3	*
73	80	N-HEXANE	341.90	1.01	35	*
75	80	N-HEXANE	343.20	1.03	6	*
75	80	N-HEXANE	333.20	1.04	3	*
75	80	N-HEXANE	341.90	0.95	35	*
75	80	N-HEXANE	340.80	1.05	3	*
81	80	N-HEXANE	348.20	1.01	3	*
83	80	N-HEXANE	298.20	1.01	3	*
83	80	N-HEXANE	133.70	1.03	3	*
83	80	N-HEXANE	340.70	1.06	3	*
83	80	N-HEXANE	348.20	1.57	3	*
83	80	N-HEXANE	341.90	1.38	3	*
84	80	N-HEXANE	341.90	1.00	3	*
103	80	N-HEXANE	341.90	1.48	3	*
133	80	N-HEXANE	333.20	0.83	3	*
133	80	N-HEXANE	293.20	0.92	3	*
2	81	2,3-DIMETHYL BUTANE	331.00	1.22	3	*
4	81	2,3-DIMETHYL BUTANE	331.00	1.47	3	*
66	81	2,3-DIMETHYL BUTANE	323.20	1.63	3	*
66	81	2,3-DIMETHYL BUTANE	283.20	2.06	3	*
80	81	2,3-DIMETHYL BUTANE	298.20	1.00	3	*
133	81	2,3-DIMETHYL BUTANE	293.20	0.87	3	*
96	81	2,3-DIMETHYL BUTANE	298.20	1.21	3	*
105	81	2,3-DIMETHYL BUTANE	298.20	1.32	3	*
91	82	3-METHYL PENTANE	283.20	1.82	3	*
91	82	3-METHYL PENTANE	323.20	1.59	3	*
133	82	3-METHYL PENTANE	293.20	0.90	3	*
66	83	2,2-DIMETHYL BUTANE	323.20	1.61	3	*
80	83	2,2-DIMETHYL BUTANE	298.20	0.98	3	*
133	83	2,2-DIMETHYL BUTANE	293.20	0.86	3	*
2	85	2-METHYL PENTANE	333.60	1.24	3	*
66	85	2-METHYL PENTANE	323.20	1.59	3	*
66	85	2-METHYL PENTANE	283.20	2.03	3	*
133	85	2-METHYL PENTANE	293.20	0.81	3	*
72	86	N-HEXANOL	343.20	2.59	3	*
72	86	N-HEXANOL	323.20	3.10	3	*
103	86	N-HEXANOL	430.20	1.92	3	*
8	87	TRIETHYLAMINE	362.25	2.24	41	*
19	87	TRIETHYLAMINE	311.60	1.82	40	*

SLT	SLV	SOLVENT	TEMP	GAMMA	INF.	REF
19	87	TRIETHYLAMINE	308.20	1.87	3	*
31	87	TRIETHYLAMINE	283.20	1.19	3	*
56	87	TRIETHYLAMINE	333.20	1.17	3	*
73	87	TRIETHYLAMINE	333.20	1.01	3	*
80	87	TRIETHYLAMINE	333.20	1.03	3	*
98	87	TRIETHYLAMINE	333.20	1.03	3	*
91	88	BENZONITRILE	298.20	1.50	3	*
109	88	BENZONITRILE	298.20	8.52	3	*
2	91	TOLUENE	318.20	1.03	3	*
2	91	TOLUENE	383.80	7.50	45	*
8	91	TOLUENE	383.60	6.85	3	*
11	91	TOLUENE	343.20	3.56	12	*
11	91	TOLUENE	303.20	2.83	12	*
11	91	TOLUENE	293.20	4.14	12	*
14	91	TOLUENE	383.60	1.01	3	*
16	91	TOLUENE	318.20	2.44	3	*
19	91	TOLUENE	308.20	11.70	8	*
19	91	TOLUENE	323.20	9.18	3	*
19	91	TOLUENE	383.60	5.28	3	*
20	91	TOLUENE	308.20	2.52	3	*
20	91	TOLUENE	298.20	2.48	3	*
21	91	TOLUENE	318.20	1.72	3	*
21	91	TOLUENE	308.20	1.95	3	*
21	91	TOLUENE	328.20	1.66	3	*
31	91	TOLUENE	383.60	3.97	3	*
32	91	TOLUENE	323.20	1.47	3	*
37	91	TOLUENE	353.20	1.21	3	*
43	91	TOLUENE	383.60	3.58	3	*
44	91	TOLUENE	293.20	1.67	3	*
44	91	TOLUENE	313.20	1.58	3	*
44	91	TOLUENE	383.60	1.30	3	*
56	91	TOLUENE	323.20	1.10	3	*
63	91	TOLUENE	363.20	3.23	3	*
64	91	TOLUENE	373.20	1.87	3	*
65	91	TOLUENE	303.20	0.96	3	*
65	91	TOLUENE	343.20	0.97	3	*
66	91	TOLUENE	383.70	1.02	43	*
66	91	TOLUENE	293.15	0.99	42	*
67	91	TOLUENE	383.60	2.79	3	*
68	91	TOLUENE	353.20	2.50	44	*
68	91	TOLUENE	303.20	3.27	3	*
68	91	TOLUENE	363.20	2.28	44	*
68	91	TOLUENE	373.20	2.24	44	*
72	91	TOLUENE	383.60	1.24	3	*
72	91	TOLUENE	348.20	1.40	26	*
72	91	TOLUENE	298.20	1.63	26	*
72	91	TOLUENE	293.20	1.62	3	*
72	91	TOLUENE	383.70	1.33	43	*

SLT	SLV		TEMP	GAMMA	REF	
	ID	SOLVENT		INF.		
10						
73	91	TOLUENE	283.20	1.34	3	*
73	91	TOLUENE	323.20	1.25	3	*
75	91	TOLUENE	298.20	1.53	26	*
75	91	TOLUENE	348.20	1.35	26	*
75	91	TOLUENE	383.60	1.27	3	*
80	91	TOLUENE	298.20	1.76	26	*
80	91	TOLUENE	348.20	1.55	26	*
80	91	TOLUENE	383.60	1.38	3	*
82	91	TOLUENE	323.20	1.53	3	*
88	91	TOLUENE	383.60	1.15	3	*
94	91	TOLUENE	348.20	1.25	26	*
94	91	TOLUENE	333.20	1.37	3	*
94	91	TOLUENE	298.20	1.42	26	*
98	91	TOLUENE	348.20	1.33	26	*
98	91	TOLUENE	383.60	1.34	3	*
98	91	TOLUENE	298.20	1.57	26	*
103	91	TOLUENE	383.70	1.06	43	*
108	91	TOLUENE	383.60	1.41	3	*
108	91	TOLUENE	363.15	1.34	39	*
109	91	TOLUENE	363.15	1.37	39	*
109	91	TOLUENE	383.60	1.36	3	*
8	92	ANISOLE	427.00	3.34	3	*
16	94	METHYL CYCLOHEXANE	318.20	15.80	3	*
19	94	METHYL CYCLOHEXANE	328.20	23.80	3	*
31	94	METHYL CYCLOHEXANE	374.10	7.08	3	*
61	94	METHYL CYCLOHEXANE	374.20	1.06	3	*
66	94	METHYL CYCLOHEXANE	374.10	1.21	3	*
66	94	METHYL CYCLOHEXANE	298.20	1.76	26	*
66	94	METHYL CYCLOHEXANE	348.20	1.47	26	*
68	94	METHYL CYCLOHEXANE	363.20	8.77	3	*
68	94	METHYL CYCLOHEXANE	373.20	7.63	3	*
68	94	METHYL CYCLOHEXANE	353.20	10.00	3	*
80	94	METHYL CYCLOHEXANE	343.20	1.10	3	*
91	94	METHYL CYCLOHEXANE	353.20	1.31	3	*
91	94	METHYL CYCLOHEXANE	373.20	1.25	3	*
91	94	METHYL CYCLOHEXANE	298.20	1.57	26	*
91	94	METHYL CYCLOHEXANE	348.20	1.38	26	*
98	94	METHYL CYCLOHEXANE	374.20	1.02	3	*
108	94	METHYL CYCLOHEXANE	374.00	1.01	3	*
102	94	METHYL CYCLOHEXANE	313.20	1.41	3	*
102	94	METHYL CYCLOHEXANE	353.20	1.34	3	*
37	95	1-HEPTENE	353.20	2.11	3	*
41	95	1-HEPTENE	348.20	1.40	3	*
98	95	1-HEPTENE	328.20	1.08	3	*
83	96	CYCLOHEPTANE	298.20	1.24	3	*
61	97	ETHYL BUTYL KETONE	363.20	1.80	19	*
61	97	ETHYL BUTYL KETONE	333.20	2.10	19	*
98	97	ETHYL BUTYL KETONE	333.20	2.30	19	*

SLT	SLV		TEMP	GAMMA	REF	
ID	ID	SOLVENT		INF.		
98	97	ETHYL BUTYL KETONE	363.20	1.90	19	*
126	97	ETHYL BUTYL KETONE	363.20	2.00	19	*
126	97	ETHYL BUTYL KETONE	333.20	2.45	19	*
2	98	N-HEPTANE	323.20	1.10	3	*
2	98	N-HEPTANE	371.60	1.05	3	*
4	98	N-HEPTANE	298.20	1.54	3	*
4	98	N-HEPTANE	323.20	1.37	3	*
8	98	N-HEPTANE	333.15	29.60	19	*
8	98	N-HEPTANE	373.15	11.90	19	*
11	98	N-HEPTANE	313.20	25.70	3	*
11	98	N-HEPTANE	293.20	32.00	3	*
16	98	N-HEPTANE	371.60	6.89	3	*
17	98	N-HEPTANE	303.20	2.03	3	*
19	98	N-HEPTANE	333.15	16.50	19	*
19	98	N-HEPTANE	298.20	49.00	19	*
19	98	N-HEPTANE	373.20	7.30	19	*
21	98	N-HEPTANE	373.20	3.50	19	*
21	98	N-HEPTANE	333.15	4.90	19	*
21	98	N-HEPTANE	298.20	7.40	19	*
21	98	N-HEPTANE	371.60	3.11	3	*
24	98	N-HEPTANE	371.60	6.01	3	*
25	98	N-HEPTANE	338.20	13.80	3	*
26	98	N-HEPTANE	371.60	5.03	3	*
31	98	N-HEPTANE	373.20	6.20	19	*
31	98	N-HEPTANE	348.20	10.70	3	*
31	98	N-HEPTANE	303.15	40.50	48	*
32	98	N-HEPTANE	333.20	3.50	19	*
32	98	N-HEPTANE	373.20	2.60	19	*
32	98	N-HEPTANE	298.20	4.80	19	*
37	98	N-HEPTANE	353.20	2.69	3	*
41	98	N-HEPTANE	323.20	1.42	3	*
43	98	N-HEPTANE	373.15	6.20	19	*
43	98	N-HEPTANE	333.15	13.60	19	*
43	98	N-HEPTANE	298.15	37.10	19	*
43	98	N-HEPTANE	371.60	6.34	49	*
44	98	N-HEPTANE	353.20	3.11	3	*
55	98	N-HEPTANE	353.20	2.67	3	*
55	98	N-HEPTANE	333.20	2.90	19	*
55	98	N-HEPTANE	368.20	2.58	3	*
55	98	N-HEPTANE	298.20	3.70	19	*
55	98	N-HEPTANE	373.20	2.30	19	*
56	98	N-HEPTANE	323.20	3.26	3	*
65	98	N-HEPTANE	373.20	1.52	3	*
65	98	N-HEPTANE	353.20	1.57	3	*
66	98	N-HEPTANE	298.20	1.55	19	*
66	98	N-HEPTANE	343.20	1.35	19	*
66	98	N-HEPTANE	371.60	1.30	3	*
66	98	N-HEPTANE	333.15	1.35	3	*

SLV	SLV	SOLVENT	TEMP	GAMMA	INF.	REF
66	98	N-HEPTANE	363.20	1.27	19	*
66	98	N-HEPTANE	403.20	1.19	19	*
66	98	N-HEPTANE	323.20	1.43	19	*
68	98	N-HEPTANE	324.70	13.10	3	*
72	98	N-HEPTANE	403.20	1.02	19	*
72	98	N-HEPTANE	298.20	1.13	19	*
72	98	N-HEPTANE	371.60	1.05	3	*
72	98	N-HEPTANE	343.20	1.08	19	*
87	98	N-HEPTANE	333.20	1.03	3	*
91	98	N-HEPTANE	298.20	1.25	26	*
91	98	N-HEPTANE	343.20	1.33	19	*
91	98	N-HEPTANE	323.20	1.32	19	*
91	98	N-HEPTANE	371.60	1.30	3	*
91	98	N-HEPTANE	348.20	1.30	26	*
91	98	N-HEPTANE	363.20	1.25	19	*
91	98	N-HEPTANE	298.20	1.45	19	*
94	98	N-HEPTANE	371.60	1.03	3	*
97	98	N-HEPTANE	298.20	3.20	19	*
97	98	N-HEPTANE	373.20	1.80	19	*
97	98	N-HEPTANE	333.20	2.30	19	*
110	98	N-HEPTANE	373.20	5.60	19	*
110	98	N-HEPTANE	323.20	12.20	19	*
110	98	N-HEPTANE	298.20	33.50	19	*
116	98	N-HEPTANE	323.20	1.80	19	*
116	98	N-HEPTANE	373.20	1.40	19	*
116	98	N-HEPTANE	298.20	2.40	19	*
120	98	N-HEPTANE	323.20	1.55	19	*
120	98	N-HEPTANE	343.20	1.47	19	*
120	98	N-HEPTANE	298.20	1.78	19	*
120	98	N-HEPTANE	363.20	1.38	19	*
121	98	N-HEPTANE	343.20	1.50	19	*
102	98	N-HEPTANE	298.20	1.65	19	*
102	98	N-HEPTANE	363.20	1.38	19	*
102	98	N-HEPTANE	323.20	1.52	19	*
102	98	N-HEPTANE	343.20	1.43	19	*
143	98	N-HEPTANE	313.20	0.44	19	*
143	98	N-HEPTANE	298.20	0.47	19	*
143	98	N-HEPTANE	298.20	0.48	6	*
67	101	ACETOPHENONE	406.20	0.39	3	*
67	101	ACETOPHENONE	440.70	0.46	3	*
11	103	P-XYLENE	411.50	2.16	3	*
14	103	P-XYLENE	303.20	1.07	3	*
19	103	P-XYLENE	411.50	5.28	3	*
25	103	P-XYLENE	411.50	2.40	3	*
43	103	P-XYLENE	411.50	3.06	3	*
63	103	P-XYLENE	411.50	2.57	3	*
65	103	P-XYLENE	409.20	0.90	3	*
66	103	P-XYLENE	411.50	0.96	3	*

SLT	SLV		TEMP	GAMMA	REF	
ID	ID	SOLVENT		INF.		
72	103	P-XYLENE	328.20	1.35	3	*
80	103	P-XYLENE	411.50	1.48	3	*
86	103	P-XYLENE	411.50	2.27	3	*
91	103	P-XYLENE	411.10	1.03	43	*
109	103	P-XYLENE	409.20	1.27	3	*
2	104	O-XYLENE	303.20	0.87	3	*
14	104	O-XYLENE	303.20	1.05	3	*
25	104	O-XYLENE	349.00	2.83	3	*
72	104	O-XYLENE	303.20	1.50	3	*
72	104	O-XYLENE	323.20	1.43	3	*
81	105	CYCLOOCTANE	298.20	1.31	3	*
37	106	1-OCTENE	353.20	2.06	3	*
66	106	1-OCTENE	303.20	1.26	3	*
66	106	1-OCTENE	323.20	1.21	3	*
72	106	1-OCTENE	313.20	1.10	3	*
102	106	1-OCTENE	393.20	1.09	3	*
109	107	ETHYL CYCLOHEXANE	382.30	1.02	3	*
102	107	ETHYL CYCLOHEXANE	382.30	1.21	3	*
2	108	ISOOCTANE	348.20	1.14	3	*
2	108	ISOOCTANE	318.20	1.17	3	*
19	108	ISOOCTANE	313.20	27.00	3	*
44	108	ISOOCTANE	313.20	5.68	3	*
44	108	ISOOCTANE	293.20	7.54	3	*
64	108	ISOOCTANE	363.15	4.15	39	*
66	108	ISOOCTANE	308.20	1.57	3	*
66	108	ISOOCTANE	372.40	1.37	3	*
72	108	ISOOCTANE	338.20	1.02	3	*
91	108	ISOOCTANE	363.15	1.37	39	*
91	108	ISOOCTANE	372.40	1.28	3	*
94	108	ISOOCTANE	372.40	1.01	3	*
102	108	ISOOCTANE	333.20	1.49	3	*
37	109	N-OCTANE	353.20	2.49	3	*
44	109	N-OCTANE	353.20	2.87	3	*
64	109	N-OCTANE	363.20	3.88	3	*
66	109	N-OCTANE	298.20	1.73	26	*
66	109	N-OCTANE	398.80	1.31	3	*
66	109	N-OCTANE	348.20	1.43	26	*
67	109	N-OCTANE	398.80	8.89	3	*
72	109	N-OCTANE	328.20	1.03	3	*
91	109	N-OCTANE	398.80	1.21	3	*
91	109	N-OCTANE	363.15	1.32	3	*
103	109	N-OCTANE	398.80	1.23	3	*
107	109	N-OCTANE	398.80	1.00	3	*
102	109	N-OCTANE	398.80	1.22	3	*
21	110	N-OCTANOL	333.15	1.84	19	*
21	110	N-OCTANOL	298.15	2.58	19	*
21	110	N-OCTANOL	373.15	1.41	19	*
32	110	N-OCTANOL	333.15	1.78	19	*

SLT	SLV		TEMP	GAMMA	REF
ID	ID	SOLVENT		INF.	
32	110	N-OCTANOL	298.20	2.30	19 *
32	110	N-OCTANOL	373.15	1.46	19 *
55	110	N-OCTANOL	333.20	1.56	19 *
55	110	N-OCTANOL	373.20	1.24	19 *
55	110	N-OCTANOL	298.20	2.12	19 *
37	117	N-NONANE	353.20	2.20	3 *
44	117	N-NONANE	369.80	2.42	3 *
44	117	N-NONANE	353.20	2.83	3 *
64	120	N-BUTYL BENZENE	373.20	1.98	3 *
46	121	DECALIN	298.20	1.34	3 *
48	121	DECALIN	298.20	1.21	3 *
66	121	DECALIN	298.20	1.47	3 *
72	121	DECALIN	298.20	1.06	3 *
80	121	DECALIN	298.20	1.26	3 *
2	102	ETHYL BENZENE	353.20	0.96	3 *
11	102	ETHYL BENZENE	409.30	2.46	3 *
19	102	ETHYL BENZENE	409.30	3.94	3 *
31	102	ETHYL BENZENE	409.30	3.76	3 *
43	102	ETHYL BENZENE	409.30	2.96	3 *
64	102	ETHYL BENZENE	373.20	1.83	3 *
65	102	ETHYL BENZENE	293.20	0.99	3 *
68	102	ETHYL BENZENE	373.20	2.12	3 *
72	102	ETHYL BENZENE	303.20	1.31	3 *
72	102	ETHYL BENZENE	323.20	1.23	3 *
94	102	ETHYL BENZENE	353.20	1.16	3 *
94	102	ETHYL BENZENE	313.20	1.30	3 *
106	102	ETHYL BENZENE	409.30	1.28	3 *
107	102	ETHYL BENZENE	409.30	1.15	3 *
108	102	ETHYL BENZENE	333.20	1.60	3 *
109	102	ETHYL BENZENE	409.30	1.22	3 *
19	126	N-DECANE	447.30	3.27	3 *
21	126	N-DECANE	298.20	6.50	19 *
21	126	N-DECANE	373.20	3.10	19 *
21	126	N-DECANE	333.20	4.50	19 *
31	126	N-DECANE	368.20	7.00	3 *
32	126	N-DECANE	373.20	2.80	19 *
32	126	N-DECANE	333.20	3.50	19 *
32	126	N-DECANE	298.20	4.80	19 *
44	126	N-DECANE	353.20	2.60	3 *
44	126	N-DECANE	373.20	2.16	3 *
44	126	N-DECANE	444.80	1.70	3 *
67	128	N-DODECANE	489.40	2.94	3 *
72	128	N-DODECANE	305.20	0.89	3 *
8	133	N-HEXADECANE	373.20	9.30	19 *
8	133	N-HEXADECANE	298.20	75.10	19 *
8	133	N-HEXADECANE	333.20	23.30	19 *
19	133	N-HEXADECANE	298.20	40.00	19 *
19	133	N-HEXADECANE	373.20	6.00	19 *

SLT	SLV			GAMMA	
ID	ID	SOLVENT	TEMP	INF.	REF
19	133	N-HEXADECANE	333.20	13.50	19 *
21	133	N-HEXADECANE	373.20	9.10	19 *
21	133	N-HEXADECANE	298.20	6.10	19 *
21	133	N-HEXADECANE	333.20	4.20	19 *
32	133	N-HEXADECANE	373.20	2.30	19 *
32	133	N-HEXADECANE	298.20	4.20	19 *
32	133	N-HEXADECANE	333.20	2.90	19 *
55	133	N-HEXADECANE	333.20	2.60	19 *
55	133	N-HEXADECANE	373.20	2.10	19 *
55	133	N-HEXADECANE	298.20	3.30	19 *
66	133	N-HEXADECANE	333.20	0.92	3 *
66	133	N-HEXADECANE	313.20	0.93	3 *
66	133	N-HEXADECANE	353.20	0.85	3 *
72	133	N-HEXADECANE	305.20	0.79	3 *
80	133	N-HEXADECANE	293.20	0.92	3 *
80	133	N-HEXADECANE	333.20	0.83	3 *
81	133	N-HEXADECANE	293.20	0.89	3 *
82	133	N-HEXADECANE	293.20	0.88	3 *
83	133	N-HEXADECANE	293.20	0.98	3 *
85	133	N-HEXADECANE	293.20	0.95	3 *
19	136	N-EICOSANE	333.20	12.00	19 *
19	136	N-EICOSANE	373.20	5.30	19 *
72	136	N-EICOSANE	312.80	0.68	3 *
98	143	N-DOOTRIACONTANE	298.20	0.71	6 *

SLT ID	SLV ID	SOLVENT	TEMP	GAMMA INFINITY	REF
9	1	CARBON DISULFIDE	298.20	34.60	4
32	1	CARBON DISULFIDE	298.20	4.90	4
37	1	CARBON DISULFIDE	298.20	1.78	4
91	1	CARBON DISULFIDE	298.20	1.21	4
109	1	CARBON DISULFIDE	298.20	1.53	4
1	2	CARBON TETRACHLORIDE	293.15	1.21	2
4	2	CARBON TETRACHLORIDE	293.20	1.16	2
6	2	CARBON TETRACHLORIDE	293.15	1.58	2
9	2	CARBON TETRACHLORIDE	293.15	15.20	2
10	2	CARBON TETRACHLORIDE	293.15	1.37	2
11	2	CARBON TETRACHLORIDE	293.15	13.40	2
17	2	CARBON TETRACHLORIDE	293.20	1.35	2
18	2	CARBON TETRACHLORIDE	293.15	1.25	2
20	2	CARBON TETRACHLORIDE	293.20	7.20	2
21	2	CARBON TETRACHLORIDE	295.79	3.15	1
21	2	CARBON TETRACHLORIDE	293.15	3.19	2
28	2	CARBON TETRACHLORIDE	293.15	1.26	2
37	2	CARBON TETRACHLORIDE	298.20	1.26	4
44	2	CARBON TETRACHLORIDE	293.15	1.85	1
46	2	CARBON TETRACHLORIDE	293.20	1.00	2
72	2	CARBON TETRACHLORIDE	293.15	1.12	2
80	2	CARBON TETRACHLORIDE	293.20	1.33	2
87	2	CARBON TETRACHLORIDE	298.20	0.83	9
9	4	CHLOROFORM	298.20	2.65	4
11	4	CHLOROFORM	298.70	1.33	1
66	4	CHLOROFORM	298.10	0.75	1
91	4	CHLOROFORM	298.20	0.77	4
9	6	DICHLOROMETHANE	298.20	1.72	4
87	6	DICHLOROMETHANE	298.20	0.94	9
91	6	DICHLOROMETHANE	298.20	0.92	4
109	6	DICHLOROMETHANE	298.20	3.27	4
9	8	METHANOL	298.20	4.78	4
32	8	METHANOL	298.20	2.16	4
37	8	METHANOL	298.20	1.92	4
66	8	METHANOL	298.15	7.50	11
80	8	METHANOL	298.15	27.00	11
91	8	METHANOL	298.20	10.80	4
109	8	METHANOL	298.20	53.80	4
1	9	NITROMETHANE	293.15	15.10	2
2	9	NITROMETHANE	293.15	8.81	2
4	9	NITROMETHANE	293.20	2.20	2
6	9	NITROMETHANE	293.15	1.68	2
10	9	NITROMETHANE	293.15	4.70	2
17	9	NITROMETHANE	293.15	6.16	2
18	9	NITROMETHANE	293.15	3.56	2
19	9	NITROMETHANE	298.20	5.20	4
28	9	NITROMETHANE	293.15	4.44	2
32	9	NITROMETHANE	298.20	1.26	4

SLT ID	SLV ID	SOLVENT	TEMP	GAMMA INFINITY	REF
40	9	NITROMETHANE	293.15	5.55	2
45	9	NITROMETHANE	293.15	6.71	2
56	9	NITROMETHANE	293.15	3.86	2
72	9	NITROMETHANE	293.15	36.80	2
80	9	NITROMETHANE	298.15	48.00	11
80	9	NITROMETHANE	293.15	58.00	2
87	9	NITROMETHANE	293.20	12.80	1
87	9	NITROMETHANE	298.20	12.30	9
91	9	NITROMETHANE	298.20	5.95	4
108	9	NITROMETHANE	298.20	120.50	4
1	11	ACETONITRILE	293.20	12.40	2
2	11	ACETONITRILE	293.15	6.87	2
4	11	ACETONITRILE	293.20	1.49	2
10	11	ACETONITRILE	293.15	3.86	2
17	11	ACETONITRILE	293.15	5.14	2
18	11	ACETONITRILE	293.15	2.88	2
19	11	ACETONITRILE	298.20	3.39	4
21	11	ACETONITRILE	293.15	1.10	2
28	11	ACETONITRILE	293.15	3.35	2
32	11	ACETONITRILE	298.20	1.27	4
36	11	ACETONITRILE	293.20	1.58	2
37	11	ACETONITRILE	298.20	1.24	4
40	11	ACETONITRILE	293.15	4.25	2
45	11	ACETONITRILE	293.20	6.03	2
50	11	ACETONITRILE	298.20	9.47	14
61	11	ACETONITRILE	298.20	21.40	14
66	11	ACETONITRILE	298.20	3.08	14
80	11	ACETONITRILE	298.20	30.70	2
80	11	ACETONITRILE	298.15	25.50	11
87	11	ACETONITRILE	293.15	11.10	2
87	11	ACETONITRILE	298.20	10.70	9
91	11	ACETONITRILE	298.20	4.65	4
109	11	ACETONITRILE	298.20	60.30	4
1	14	1,2-DICHLOROETHANE	293.15	2.58	2
2	14	1,2-DICHLOROETHANE	293.15	1.98	2
4	14	1,2-DICHLOROETHANE	293.15	1.05	2
6	14	1,2-DICHLOROETHANE	293.15	1.02	2
10	14	1,2-DICHLOROETHANE	293.15	1.34	2
17	14	1,2-DICHLOROETHANE	293.15	1.38	2
18	14	1,2-DICHLOROETHANE	293.15	1.18	2
21	14	1,2-DICHLOROETHANE	293.15	0.75	2
28	14	1,2-DICHLOROETHANE	293.15	1.35	2
39	14	1,2-DICHLOROETHANE	293.15	1.37	2
40	14	1,2-DICHLOROETHANE	293.15	1.49	2
45	14	1,2-DICHLOROETHANE	293.15	1.68	2
48	14	1,2-DICHLOROETHANE	293.15	2.72	2
50	14	1,2-DICHLOROETHANE	293.15	2.92	2
61	14	1,2-DICHLOROETHANE	293.15	4.74	2

SLT	SLV	SOLVENT	TEMP	GAMMA INFINITY	REF
72	14	1,2-DICHLOROETHANE	293.15	3.94	2
80	14	1,2-DICHLOROETHANE	293.15	5.04	2
87	14	1,2-DICHLOROETHANE	293.20	2.14	2
87	14	1,2-DICHLOROETHANE	298.20	2.14	9
87	15	1,1-DICHLOROETHANE	298.20	0.88	9
1	16	NITROETHANE	293.15	5.03	2
2	16	NITROETHANE	293.15	3.93	2
4	16	NITROETHANE	293.15	1.00	2
6	16	NITROETHANE	293.15	0.92	2
8	16	NITROETHANE	293.15	6.07	2
17	16	NITROETHANE	293.15	2.79	2
18	16	NITROETHANE	293.15	1.70	2
19	16	NITROETHANE	298.20	5.29	4
19	16	NITROETHANE	293.15	6.73	2
28	16	NITROETHANE	293.15	1.90	2
32	16	NITROETHANE	298.20	0.94	4
37	16	NITROETHANE	298.20	1.25	4
40	16	NITROETHANE	293.15	2.32	2
46	16	NITROETHANE	293.15	2.53	2
48	16	NITROETHANE	293.15	5.06	2
50	16	NITROETHANE	293.15	5.20	2
61	16	NITROETHANE	293.15	9.62	2
66	16	NITROETHANE	293.15	1.82	2
72	16	NITROETHANE	293.15	9.61	2
80	16	NITROETHANE	293.15	11.46	2
91	16	NITROETHANE	298.20	2.43	4
108	16	NITROETHANE	293.15	18.80	2
9	18	ETHYL BROMIDE	298.20	3.85	4
108	18	ETHYL BROMIDE	298.20	1.65	4
9	19	ETHANOL	298.20	6.32	4
10	19	ETHANOL	293.15	5.26	2
17	19	ETHANOL	293.15	6.17	2
18	19	ETHANOL	293.15	4.19	2
21	19	ETHANOL	293.15	2.38	2
32	19	ETHANOL	298.20	2.25	4
37	19	ETHANOL	298.20	3.35	4
61	19	ETHANOL	293.15	9.60	2
80	19	ETHANOL	293.20	12.00	2
87	19	ETHANOL	298.20	1.26	9
109	19	ETHANOL	298.20	17.80	4
1	20	PROPIONITRILE	293.15	5.51	2
2	20	PROPIONITRILE	293.15	3.14	2
4	20	PROPIONITRILE	293.20	0.89	2
6	20	PROPIONITRILE	293.15	0.82	2
10	20	PROPIONITRILE	293.15	2.14	2
17	20	PROPIONITRILE	293.15	2.68	2
18	20	PROPIONITRILE	293.15	1.73	2
21	20	PROPIONITRILE	293.15	0.96	2

SLT	SLV		TEMP	GAMMA INFINITY	REF
	ID	SOLVENT			
28	20	PROPIONITRILE	293.15	1.87	2
36	20	PROPIONITRILE	293.20	1.44	2
39	20	PROPIONITRILE	293.20	2.64	2
40	20	PROPIONITRILE	293.15	2.37	2
46	20	PROPIONITRILE	293.15	2.57	2
48	20	PROPIONITRILE	293.15	4.51	2
50	20	PROPIONITRILE	293.15	4.57	2
61	20	PROPIONITRILE	293.15	8.53	2
66	20	PROPIONITRILE	298.15	1.58	11
66	20	PROPIONITRILE	293.20	1.84	2
72	20	PROPIONITRILE	293.15	8.40	2
80	20	PROPIONITRILE	293.15	11.00	2
80	20	PROPIONITRILE	298.15	10.20	11
87	20	PROPIONITRILE	293.15	4.40	2
94	20	PROPIONITRILE	298.20	9.98	22
98	20	PROPIONITRILE	298.20	12.20	22
32	21	ACETONE	298.20	0.94	4
37	21	ACETONE	298.20	1.37	4
66	21	ACETONE	298.15	1.70	11
80	21	ACETONE	298.15	6.50	11
91	21	ACETONE	298.20	2.15	4
2	24	1-NITROPROPANE	298.15	3.16	32
46	24	1-NITROPROPANE	298.20	2.40	32
48	24	1-NITROPROPANE	298.20	3.97	32
61	24	1-NITROPROPANE	298.20	6.64	32
66	24	1-NITROPROPANE	298.20	1.42	32
72	24	1-NITROPROPANE	298.20	5.45	32
80	24	1-NITROPROPANE	298.20	8.28	32
1	25	DIMETHYL FORMAMIDE	293.20	4.36	2
10	25	DIMETHYL FORMAMIDE	293.20	1.65	2
17	25	DIMETHYL FORMAMIDE	293.20	2.36	2
18	25	DIMETHYL FORMAMIDE	293.20	1.65	2
19	25	DIMETHYL FORMAMIDE	298.20	0.60	4
32	25	DIMETHYL FORMAMIDE	298.20	1.17	4
45	25	DIMETHYL FORMAMIDE	297.20	3.49	57
46	25	DIMETHYL FORMAMIDE	293.20	2.98	2
46	25	DIMETHYL FORMAMIDE	297.20	3.43	57
48	25	DIMETHYL FORMAMIDE	297.20	6.86	57
48	25	DIMETHYL FORMAMIDE	293.20	6.67	2
50	25	DIMETHYL FORMAMIDE	293.20	8.00	2
50	25	DIMETHYL FORMAMIDE	297.20	7.30	57
52	25	DIMETHYL FORMAMIDE	297.20	7.91	57
61	25	DIMETHYL FORMAMIDE	297.20	15.00	57
61	25	DIMETHYL FORMAMIDE	293.20	16.70	2
62	25	DIMETHYL FORMAMIDE	297.20	14.20	57
72	25	DIMETHYL FORMAMIDE	293.20	13.10	2
80	25	DIMETHYL FORMAMIDE	293.20	20.80	2
80	25	DIMETHYL FORMAMIDE	298.20	17.90	37

SLT	SLV	SOLVENT	TEMP	GAMMA INFINITY	REF
87	25	DIMETHYL FORMAMIDE	298.20	8.53	9
91	25	DIMETHYL FORMAMIDE	298.20	2.20	4
94	25	DIMETHYL FORMAMIDE	293.20	16.40	2
98	25	DIMETHYL FORMAMIDE	293.20	26.50	2
108	25	DIMETHYL FORMAMIDE	293.20	30.10	2
109	25	DIMETHYL FORMAMIDE	298.20	29.70	4
1	26	2-NITROPROPANE	293.15	4.03	2
2	26	2-NITROPROPANE	293.15	2.40	2
4	26	2-NITROPROPANE	293.15	0.88	2
6	26	2-NITROPROPANE	293.15	0.91	2
8	26	2-NITROPROPANE	293.15	8.35	2
10	26	2-NITROPROPANE	293.15	2.03	2
17	26	2-NITROPROPANE	293.15	2.22	2
18	26	2-NITROPROPANE	293.15	1.53	2
19	26	2-NITROPROPANE	293.15	8.42	2
28	26	2-NITROPROPANE	293.15	1.64	2
46	26	2-NITROPROPANE	293.15	2.10	2
48	26	2-NITROPROPANE	293.20	3.41	2
50	26	2-NITROPROPANE	293.15	3.67	2
61	26	2-NITROPROPANE	293.15	6.50	2
72	26	2-NITROPROPANE	293.15	5.70	2
80	26	2-NITROPROPANE	293.15	7.50	2
94	26	2-NITROPROPANE	293.15	6.80	2
98	26	2-NITROPROPANE	293.15	8.81	2
9	31	N-PROPANOL	298.20	8.16	4
32	31	N-PROPANOL	298.20	2.41	4
37	31	N-PROPANOL	298.20	2.93	4
87	31	N-PROPANOL	298.20	0.90	9
91	31	N-PROPANOL	298.20	4.59	4
109	31	N-PROPANOL	298.20	10.70	4
1	32	2-BUTANONE	293.15	3.04	2
2	32	2-BUTANONE	293.15	1.65	2
6	32	2-BUTANONE	293.15	0.51	2
10	32	2-BUTANONE	293.15	1.45	2
17	32	2-BUTANONE	293.15	1.58	2
18	32	2-BUTANONE	293.15	1.14	2
21	32	2-BUTANONE	293.15	1.05	2
28	32	2-BUTANONE	293.15	1.18	2
37	32	2-BUTANONE	298.20	1.22	4
40	32	2-BUTANONE	293.15	1.45	2
46	32	2-BUTANONE	293.15	1.50	2
48	32	2-BUTANONE	293.15	2.36	2
50	32	2-BUTANONE	293.15	2.52	2
61	32	2-BUTANONE	293.20	3.66	2
80	32	2-BUTANONE	293.15	4.30	2
87	32	2-BUTANONE	293.15	2.79	2
87	32	2-BUTANONE	298.20	2.74	9
91	32	2-BUTANONE	298.20	1.42	4

SLT	SLV	SOLVENT	TEMP	GAMMA INFINITY	REF
109	32	2-BUTANONE	298.20	5.83	4
6	34	TETRAHYDROFURAN	293.70	0.41	1
37	34	TETRAHYDROFURAN	298.20	1.06	4
87	34	TETRAHYDROFURAN	298.20	1.44	9
1	36	ETHYL ACETATE	293.15	2.66	2
2	36	ETHYL ACETATE	293.15	1.31	2
6	36	ETHYL ACETATE	293.15	0.49	2
10	36	ETHYL ACETATE	293.15	1.34	2
17	36	ETHYL ACETATE	293.15	1.55	2
18	36	ETHYL ACETATE	293.15	1.04	2
21	36	ETHYL ACETATE	293.15	1.13	2
28	36	ETHYL ACETATE	293.15	1.10	2
37	36	ETHYL ACETATE	298.20	1.09	4
40	36	ETHYL ACETATE	293.20	1.21	2
46	36	ETHYL ACETATE	293.15	1.33	2
48	36	ETHYL ACETATE	293.15	2.05	2
50	36	ETHYL ACETATE	293.15	2.05	2
61	36	ETHYL ACETATE	293.15	3.09	2
72	36	ETHYL ACETATE	293.15	3.24	2
80	36	ETHYL ACETATE	293.15	3.49	2
87	36	ETHYL ACETATE	293.15	2.43	2
87	36	ETHYL ACETATE	298.20	2.46	9
91	36	ETHYL ACETATE	298.20	1.33	4
109	36	ETHYL ACETATE	298.20	4.75	4
32	37	DIOXANE	298.20	1.33	4
87	37	DIOXANE	298.20	3.38	9
91	37	DIOXANE	298.20	1.51	4
1	39	N-BUTYL CHLORIDE	293.15	1.56	2
4	39	N-BUTYL CHLORIDE	293.20	0.93	2
6	39	N-BUTYL CHLORIDE	293.15	1.02	2
9	39	N-BUTYL CHLORIDE	293.20	5.40	2
10	39	N-BUTYL CHLORIDE	293.15	1.31	2
17	39	N-BUTYL CHLORIDE	293.20	1.29	2
18	39	N-BUTYL CHLORIDE	293.15	1.02	2
21	39	N-BUTYL CHLORIDE	293.15	1.60	2
28	39	N-BUTYL CHLORIDE	293.15	1.02	2
40	39	N-BUTYL CHLORIDE	293.15	1.00	2
72	39	N-BUTYL CHLORIDE	293.20	1.62	2
80	39	N-BUTYL CHLORIDE	293.20	1.73	2
1	43	N-BUTANOL	293.15	3.14	2
2	43	N-BUTANOL	293.15	2.67	2
4	43	N-BUTANOL	293.15	1.20	2
6	43	N-BUTANOL	293.15	1.86	2
9	43	N-BUTANOL	293.15	9.10	2
10	43	N-BUTANOL	293.15	3.05	2
11	43	N-BUTANOL	293.15	5.67	2
14	43	N-BUTANOL	293.15	2.92	2
17	43	N-BUTANOL	293.15	3.44	2

SLT	SLV	SOLVENT	TEMP	GAMMA INFINITY	REF
18	43	N-BUTANOL	293.15	2.66	2
20	43	N-BUTANOL	293.15	5.20	2
21	43	N-BUTANOL	298.20	2.52	2
21	43	N-BUTANOL	293.20	2.40	2
28	43	N-BUTANOL	293.15	2.88	2
32	43	N-BUTANOL	298.15	2.06	4
46	43	N-BUTANOL	293.15	2.91	2
48	43	N-BUTANOL	293.15	3.43	2
50	43	N-BUTANOL	293.15	3.54	2
61	43	N-BUTANOL	298.20	4.06	36
61	43	N-BUTANOL	293.15	4.30	2
66	43	N-BUTANOL	298.20	2.84	36
72	43	N-BUTANOL	298.20	3.74	36
72	43	N-BUTANOL	293.15	4.01	2
80	43	N-BUTANOL	293.15	5.00	2
91	43	N-BUTANOL	298.20	3.54	4
98	43	N-BUTANOL	293.15	7.00	2
109	43	N-BUTANOL	298.20	7.96	37
9	44	PYRIDINE	298.20	1.23	4
19	44	PYRIDINE	298.15	1.10	4
32	44	PYRIDINE	298.20	1.01	4
37	44	PYRIDINE	298.20	1.10	4
66	44	PYRIDINE	298.15	1.20	11
80	44	PYRIDINE	298.15	6.20	11
91	44	PYRIDINE	298.20	1.49	4
109	44	PYRIDINE	298.20	8.32	4
1	64	NITROBENZENE	293.15	2.63	2
2	64	NITROBENZENE	293.15	2.26	2
4	64	NITROBENZENE	293.15	1.02	2
6	64	NITROBENZENE	293.15	0.99	2
8	64	NITROBENZENE	293.15	10.40	2
9	64	NITROBENZENE	298.20	1.39	4
10	64	NITROBENZENE	293.15	1.68	2
11	64	NITROBENZENE	293.15	1.73	2
14	64	NITROBENZENE	293.15	1.09	2
17	64	NITROBENZENE	293.15	1.83	2
18	64	NITROBENZENE	293.15	1.50	2
19	64	NITROBENZENE	293.15	10.70	2
19	64	NITROBENZENE	298.20	7.26	4
21	64	NITROBENZENE	293.15	1.24	2
28	64	NITROBENZENE	293.15	1.81	2
32	64	NITROBENZENE	298.20	1.11	4
36	64	NITROBENZENE	293.15	1.38	2
37	64	NITROBENZENE	298.20	0.96	4
40	64	NITROBENZENE	293.15	2.41	2
46	64	NITROBENZENE	298.20	2.40	36
46	64	NITROBENZENE	293.15	2.40	2
48	64	NITROBENZENE	293.15	3.72	2

SLT	SLV	SOLVENT	TEMP	GAMMA INFINITY	REF
48	64	NITROBENZENE	298.20	3.48	36
50	64	NITROBENZENE	293.15	4.49	2
61	64	NITROBENZENE	293.15	7.46	2
61	64	NITROBENZENE	298.20	7.02	36
66	64	NITROBENZENE	298.20	1.39	36
66	64	NITROBENZENE	298.20	1.41	37
66	64	NITROBENZENE	293.15	1.39	2
72	64	NITROBENZENE	298.20	5.79	36
80	64	NITROBENZENE	298.20	7.81	36
80	64	NITROBENZENE	298.20	8.24	37
80	64	NITROBENZENE	293.15	8.20	2
87	64	NITROBENZENE	298.20	3.60	9
87	64	NITROBENZENE	293.15	4.05	2
91	64	NITROBENZENE	293.20	1.69	4
94	64	NITROBENZENE	293.15	7.22	2
98	64	NITROBENZENE	298.20	8.70	36
98	64	NITROBENZENE	293.15	9.40	2
108	64	NITROBENZENE	293.20	11.80	2
109	64	NITROBENZENE	298.20	11.30	4
1	65	CHLOROBENZENE	293.15	1.26	2
2	65	CHLOROBENZENE	293.15	1.01	2
4	65	CHLOROBENZENE	293.15	0.89	2
6	65	CHLOROBENZENE	293.15	1.03	2
8	65	CHLOROBENZENE	293.15	23.30	2
9	65	CHLOROBENZENE	298.20	3.69	4
9	65	CHLOROBENZENE	293.15	3.48	2
10	65	CHLOROBENZENE	293.15	1.07	2
11	65	CHLOROBENZENE	293.15	3.11	2
17	65	CHLOROBENZENE	293.15	1.00	2
18	65	CHLOROBENZENE	293.15	0.96	2
19	65	CHLOROBENZENE	293.15	18.20	2
21	65	CHLOROBENZENE	293.15	1.42	2
28	65	CHLOROBENZENE	293.15	1.01	2
32	65	CHLOROBENZENE	298.20	1.00	4
36	65	CHLOROBENZENE	293.15	0.92	2
37	65	CHLOROBENZENE	298.20	0.98	4
40	65	CHLOROBENZENE	293.15	1.21	2
46	65	CHLOROBENZENE	293.15	1.19	2
48	65	CHLOROBENZENE	293.15	1.47	2
50	65	CHLOROBENZENE	293.15	1.60	2
61	65	CHLOROBENZENE	293.15	2.02	2
66	65	CHLOROBENZENE	293.15	0.86	2
72	65	CHLOROBENZENE	293.15	1.71	2
80	65	CHLOROBENZENE	293.15	1.98	2
91	65	CHLOROBENZENE	298.20	1.02	4
109	65	CHLOROBENZENE	298.20	2.16	4
1	66	BENZENE	293.15	1.48	2
2	66	BENZENE	293.15	1.13	1

SLT ID	SLV ID	SOLVENT	TEMP	GAMMA INFINITY	REF
4	66	BENZENE	293.20	0.67	2
6	66	BENZENE	293.15	0.77	2
10	66	BENZENE	293.15	1.15	2
11	66	BENZENE	293.15	3.47	2
17	66	BENZENE	293.15	1.12	2
18	66	BENZENE	293.15	1.01	2
21	66	BENZENE	293.15	1.71	2
28	66	BENZENE	293.15	1.06	2
32	66	BENZENE	298.20	1.17	4
37	66	BENZENE	298.20	0.89	4
40	66	BENZENE	293.15	1.27	2
46	66	BENZENE	293.15	1.24	2
48	66	BENZENE	293.15	1.67	2
50	66	BENZENE	293.15	1.72	2
61	66	BENZENE	293.15	2.25	2
72	66	BENZENE	293.15	1.69	2
80	66	BENZENE	293.15	2.21	2
87	66	BENZENE	298.20	1.30	9
91	66	BENZENE	298.20	0.93	4
109	66	BENZENE	298.20	1.79	4
46	67	PHENOL	298.20	4.64	36
48	67	PHENOL	298.20	6.92	36
61	67	PHENOL	298.20	12.70	36
66	67	PHENOL	298.20	2.57	36
80	67	PHENOL	298.20	15.20	36
98	67	PHENOL	298.20	18.80	36
1	68	ANILINE	293.20	3.53	2
2	68	ANILINE	293.20	4.80	2
4	68	ANILINE	293.20	1.50	2
6	68	ANILINE	293.20	1.41	2
8	68	ANILINE	293.20	2.39	2
9	68	ANILINE	298.20	1.11	4
17	68	ANILINE	293.20	2.83	2
18	68	ANILINE	293.20	2.14	2
21	68	ANILINE	293.20	0.80	2
36	68	ANILINE	293.20	1.44	2
40	68	ANILINE	293.20	4.82	2
46	68	ANILINE	293.20	5.27	2
46	68	ANILINE	298.20	4.90	36
47	68	ANILINE	293.20	9.18	46
48	68	ANILINE	298.20	9.00	36
48	68	ANILINE	293.20	8.61	2
50	68	ANILINE	293.20	10.40	2
61	68	ANILINE	293.20	20.10	2
61	68	ANILINE	293.20	19.72	46
61	68	ANILINE	298.20	18.40	36
62	68	ANILINE	293.20	20.29	46
66	68	ANILINE	298.20	2.08	36

SLT	SLV		TEMP	GAMMA INFINITY	REF
10	68	ANILINE	298.20	2.24	37
66	68	ANILINE	298.15	2.20	11
66	68	ANILINE	293.20	2.24	2
71	68	ANILINE	293.20	11.85	46
72	68	ANILINE	298.20	11.90	36
72	68	ANILINE	293.20	13.62	11
72	68	ANILINE	293.20	12.99	46
73	68	ANILINE	293.20	12.50	46
76	68	ANILINE	293.20	12.29	46
80	68	ANILINE	293.20	25.70	2
80	68	ANILINE	298.15	25.00	11
80	68	ANILINE	298.20	26.63	37
80	68	ANILINE	298.20	23.10	36
80	68	ANILINE	293.20	24.87	46
91	68	ANILINE	298.20	3.18	4
94	68	ANILINE	293.20	17.53	46
95	68	ANILINE	293.20	15.84	46
98	68	ANILINE	293.20	31.77	46
98	68	ANILINE	298.20	28.50	36
108	68	ANILINE	293.20	39.43	46
109	68	ANILINE	298.20	40.60	4
1	70	CYCLOHEXANONE	293.15	1.87	2
2	70	CYCLOHEXANONE	293.15	1.10	2
4	70	CYCLOHEXANONE	293.15	0.31	2
6	70	CYCLOHEXANONE	293.15	0.39	2
10	70	CYCLOHEXANONE	293.15	1.05	2
11	70	CYCLOHEXANONE	293.15	1.43	2
17	70	CYCLOHEXANONE	293.15	1.13	2
18	70	CYCLOHEXANONE	293.15	0.96	2
19	70	CYCLOHEXANONE	298.20	1.79	4
21	70	CYCLOHEXANONE	293.15	1.26	2
28	70	CYCLOHEXANONE	293.15	1.06	2
32	70	CYCLOHEXANONE	298.20	1.08	4
36	70	CYCLOHEXANONE	293.15	1.26	2
37	70	CYCLOHEXANONE	298.20	1.20	4
40	70	CYCLOHEXANONE	293.15	1.31	2
46	70	CYCLOHEXANONE	293.15	1.48	2
46	70	CYCLOHEXANONE	298.20	1.34	32
48	70	CYCLOHEXANONE	293.15	2.43	2
48	70	CYCLOHEXANONE	298.20	2.09	32
50	70	CYCLOHEXANONE	293.15	2.59	2
61	70	CYCLOHEXANONE	298.20	3.35	32
61	70	CYCLOHEXANONE	293.15	3.97	2
62	70	CYCLOHEXANONE	298.20	3.34	32
66	70	CYCLOHEXANONE	293.15	0.93	2
66	70	CYCLOHEXANONE	298.20	0.80	32
72	70	CYCLOHEXANONE	293.15	3.08	2
72	70	CYCLOHEXANONE	298.20	2.50	32

SLT	SLV		TEMP	GAMMA INFINITY	REF
80	70	CYCLOHEXANONE	298.20	3.69	32
80	70	CYCLOHEXANONE	293.15	4.46	2
87	70	CYCLOHEXANONE	293.15	2.59	2
91	70	CYCLOHEXANONE	298.20	1.26	4
109	70	CYCLOHEXANONE	298.20	5.75	4
9	72	CYCLOHEXANE	298.20	40.50	4
19	72	CYCLOHEXANE	298.20	36.30	4
32	72	CYCLOHEXANE	298.20	5.10	4
37	72	CYCLOHEXANE	298.20	4.29	4
87	72	CYCLOHEXANE	298.20	1.03	9
91	72	CYCLOHEXANE	298.20	1.55	4
109	72	CYCLOHEXANE	298.20	0.91	4
31	14	1,2-DICHLOROETHANE	303.20	8.14	17
91	14	1,2-DICHLOROETHANE	303.20	1.12	17
73	64	NITROBENZENE	303.20	4.81	38
69	64	NITROBENZENE	303.20	3.03	38
80	64	NITROBENZENE	303.20	7.70	38
72	64	NITROBENZENE	303.20	5.61	38
66	64	NITROBENZENE	303.20	1.37	38
80	67	PHENOL	303.20	14.10	38
72	67	PHENOL	303.20	7.67	38
73	67	PHENOL	303.20	7.75	38
69	67	PHENOL	303.20	4.35	38
69	68	ANILINE	303.20	6.00	38
80	68	ANILINE	303.20	22.80	38
66	68	ANILINE	303.20	2.18	38
72	68	ANILINE	303.20	12.00	38
73	68	ANILINE	303.20	11.70	38
73	78	CYCLOHEXANOL	303.20	4.72	38
72	78	CYCLOHEXANOL	303.20	3.37	38
69	78	CYCLOHEXANOL	303.20	2.78	38
66	78	CYCLOHEXANOL	303.20	2.71	38
80	78	CYCLOHEXANOL	303.20	5.65	38
21	2	CARBON TETRACHLORIDE	303.86	3.03	1
2	21	ACETONE	304.00	2.16	1
66	21	ACETONE	304.03	1.59	1
80	14	1,2-DICHLOROETHANE	304.50	4.40	1
87	21	ACETONE	304.70	3.95	1
34	4	CHLOROFORM	305.00	0.21	1
21	4	CHLOROFORM	305.00	0.39	1
18	4	CHLOROFORM	305.00	0.82	1
21	19	ETHANOL	305.20	2.14	2
87	36	ETHYL ACETATE	306.20	2.04	1
19	21	ACETONE	306.83	2.24	1
2	14	1,2-DICHLOROETHANE	306.90	1.86	1
17	36	ETHYL ACETATE	307.20	1.50	1
66	67	PHENOL	307.20	2.49	36
46	67	PHENOL	307.20	4.47	36

SLT	SLV		TEMP	GAMMA INFINITY	REF
10	10	SOLVENT			
98	67	PHENOL	307.20	17.30	36
61	67	PHENOL	307.20	12.00	36
48	67	PHENOL	307.20	6.59	36
80	67	PHENOL	307.20	14.20	36
61	68	ANILINE	307.20	17.40	36
98	68	ANILINE	307.20	26.50	36
46	68	ANILINE	307.20	4.86	36
48	68	ANILINE	307.20	8.58	36
66	68	ANILINE	307.20	2.14	36
72	68	ANILINE	307.20	11.30	36
80	68	ANILINE	307.20	21.50	36
17	21	ACETONE	307.90	2.18	1
61	11	ACETONITRILE	308.20	18.80	14
50	11	ACETONITRILE	308.20	8.58	14
80	36	ETHYL ACETATE	308.20	3.09	1
4	21	ACETONE	308.32	0.53	1
21	39	N-BUTYL CHLORIDE	309.50	1.62	1
66	72	CYCLOHEXANE	310.87	1.48	1
2	21	ACETONE	310.88	2.13	1
87	14	1,2-DICHLOROETHANE	310.90	2.05	1
87	39	N-BUTYL CHLORIDE	311.40	1.14	2
6	34	TETRAHYDROFURAN	311.45	0.45	1
20	36	ETHYL ACETATE	311.60	1.42	1
66	36	ETHYL ACETATE	311.65	1.14	1
9	36	ETHYL ACETATE	311.70	1.62	2
14	36	ETHYL ACETATE	311.70	0.81	1
11	36	ETHYL ACETATE	311.70	1.73	2
91	36	ETHYL ACETATE	313.00	1.27	1
32	36	ETHYL ACETATE	313.00	1.11	1
34	36	ETHYL ACETATE	313.00	1.10	1
8	21	ACETONE	313.15	1.90	21
91	14	1,2-DICHLOROETHANE	313.20	1.09	17
31	14	1,2-DICHLOROETHANE	313.20	6.59	17
50	25	DIMETHYL FORMAMIDE	313.20	6.56	57
61	25	DIMETHYL FORMAMIDE	313.20	12.80	57
48	25	DIMETHYL FORMAMIDE	313.20	6.11	57
46	25	DIMETHYL FORMAMIDE	313.20	3.10	57
45	25	DIMETHYL FORMAMIDE	313.20	3.06	57
62	25	DIMETHYL FORMAMIDE	313.20	12.50	57
52	25	DIMETHYL FORMAMIDE	313.20	6.74	57
44	2	CARBON TETRACHLORIDE	314.00	1.83	1
66	21	ACETONE	314.43	1.57	1
72	66	BENZENE	314.57	1.61	1
18	32	2-BUTANONE	314.70	1.05	1
36	32	2-BUTANONE	314.70	1.11	1
19	32	2-BUTANONE	314.70	2.26	1
14	32	2-BUTANONE	314.70	0.77	1
94	32	2-BUTANONE	314.70	3.80	1

SLT	SLV	SOLVENT	TEMP	GAMMA INFINITY	REF
11	32	2-BUTANONE	314.70	1.25	1
8	32	2-BUTANONE	314.70	2.29	1
9	32	2-BUTANONE	314.70	1.25	1
11	2	CARBON TETRACHLORIDE	314.90	10.70	1
9	2	CARBON TETRACHLORIDE	314.90	11.70	1
26	2	CARBON TETRACHLORIDE	314.90	4.58	1
32	2	CARBON TETRACHLORIDE	314.90	2.10	1
39	72	CYCLOHEXANE	315.08	1.56	1
19	21	ACETONE	315.16	2.12	1
2	14	1,2-DICHLOROETHANE	315.40	1.79	1
17	21	ACETONE	315.40	2.13	1
87	21	ACETONE	315.50	3.73	1
44	11	ACETONITRILE	315.80	1.92	1
44	2	CARBON TETRACHLORIDE	315.90	1.81	1
8	4	CHLOROFORM	316.00	6.93	1
19	4	CHLOROFORM	316.00	4.49	1
87	32	2-BUTANONE	316.00	2.48	1
21	2	CARBON TETRACHLORIDE	316.50	2.88	1
11	2	CARBON TETRACHLORIDE	316.50	10.10	1
72	2	CARBON TETRACHLORIDE	317.90	1.11	1
98	66	BENZENE	317.99	1.92	1
66	43	N-BUTANOL	318.15	3.01	2
66	11	ACETONITRILE	318.16	2.95	1
66	11	ACETONITRILE	318.20	2.83	14
91	11	ACETONITRILE	318.20	3.90	14
61	11	ACETONITRILE	318.20	16.60	14
9	66	BENZENE	318.21	3.48	1
11	66	BENZENE	318.22	3.08	1
19	14	1,2-DICHLOROETHANE	318.40	9.70	1
8	14	1,2-DICHLOROETHANE	318.40	9.10	1
66	14	1,2-DICHLOROETHANE	318.40	1.08	1
36	14	1,2-DICHLOROETHANE	318.40	0.83	1
21	14	1,2-DICHLOROETHANE	318.50	0.76	1
32	14	1,2-DICHLOROETHANE	318.50	0.73	1
2	14	1,2-DICHLOROETHANE	318.50	1.76	1
98	14	1,2-DICHLOROETHANE	318.50	4.45	1
9	14	1,2-DICHLOROETHANE	318.50	1.86	1
11	14	1,2-DICHLOROETHANE	318.50	1.47	1
20	14	1,2-DICHLOROETHANE	318.50	1.15	1
16	14	1,2-DICHLOROETHANE	318.50	1.49	1
91	19	ETHANOL	318.51	5.80	1
80	14	1,2-DICHLOROETHANE	319.00	3.99	1
98	19	ETHANOL	319.42	11.80	1
11	4	CHLOROFORM	319.80	1.32	1
80	4	CHLOROFORM	319.80	1.79	1
9	4	CHLOROFORM	319.80	2.90	1
66	4	CHLOROFORM	319.80	0.83	1
21	2	CARBON TETRACHLORIDE	320.76	2.85	1

SLT	SLV	SOLVENT	TEMP	GAMMA INFINITY	REF
87	36	ETHYL ACETATE	321.20	1.94	1
21	19	ETHANOL	322.51	2.17	1
18	4	CHLOROFORM	323.00	0.83	1
34	4	CHLOROFORM	323.00	0.25	1
21	4	CHLOROFORM	323.00	0.48	1
87	4	CHLOROFORM	323.00	0.27	1
8	21	ACETONE	323.15	1.80	21
61	11	ACETONITRILE	323.20	15.80	14
98	11	ACETONITRILE	323.20	27.50	14
31	14	1,2-DICHLOROETHANE	323.20	5.27	17
94	67	PHENOL	323.20	10.20	2
4	67	PHENOL	323.20	1.75	2
28	67	PHENOL	323.20	2.68	2
18	67	PHENOL	323.20	2.05	2
6	67	PHENOL	323.20	1.71	2
2	67	PHENOL	323.20	3.40	2
98	67	PHENOL	323.20	15.50	2
91	67	PHENOL	323.20	2.62	2
10	67	PHENOL	323.20	2.33	2
80	67	PHENOL	323.20	13.00	2
66	67	PHENOL	323.20	2.32	2
72	67	PHENOL	323.20	7.20	2
1	67	PHENOL	323.20	3.20	2
14	67	PHENOL	323.20	1.72	2
61	67	PHENOL	323.20	10.90	2
17	67	PHENOL	323.20	2.40	2
72	70	CYCLOHEXANONE	323.20	2.58	4
65	19	ETHANOL	323.21	5.20	1
91	14	1,2-DICHLOROETHANE	323.30	1.06	17
44	20	PROPIONITRILE	323.30	1.36	1
21	2	CARBON TETRACHLORIDE	323.31	2.80	1
80	36	ETHYL ACETATE	324.40	2.77	1
27	19	ETHANOL	325.10	6.56	1
39	72	CYCLOHEXANE	325.81	1.52	1
2	21	ACETONE	326.00	2.15	1
17	21	ACETONE	326.40	2.04	1
87	21	ACETONE	326.70	3.50	1
21	39	N-BUTYL CHLORIDE	328.70	1.53	1
4	21	ACETONE	327.41	0.58	1
19	21	ACETONE	327.41	1.92	1
2	21	ACETONE	327.60	2.13	1
4	34	TETRAHYDROFURAN	327.70	0.35	1
72	34	TETRAHYDROFURAN	327.70	1.69	1
32	2	CARBON TETRACHLORIDE	328.30	2.08	1
87	2	CARBON TETRACHLORIDE	328.30	0.75	1
98	2	CARBON TETRACHLORIDE	328.30	1.27	1
66	2	CARBON TETRACHLORIDE	328.30	1.10	1
9	2	CARBON TETRACHLORIDE	328.30	10.70	1

SLV	SLV		TEMP	GAMMA INFINITY	REF
8	4	CHLOROFORM	328.40	6.38	1
6	34	TETRAHYDROFURAN	328.40	0.48	1
87	14	1,2-DICHLOROETHANE	329.00	1.96	1
66	21	ACETONE	329.00	1.54	1
4	36	ETHYL ACETATE	329.15	0.49	1
20	36	ETHYL ACETATE	329.20	1.35	1
2	36	ETHYL ACETATE	329.20	1.28	1
44	66	BENZENE	329.70	1.21	1
91	19	ETHANOL	329.98	5.34	1
11	2	CARBON TETRACHLORIDE	330.00	9.10	1
44	14	1,2-DICHLOROETHANE	330.00	0.90	1
72	2	CARBON TETRACHLORIDE	330.40	1.10	1
66	36	ETHYL ACETATE	330.45	1.14	1
9	36	ETHYL ACETATE	330.50	1.47	2
14	36	ETHYL ACETATE	330.50	0.83	1
11	36	ETHYL ACETATE	330.50	1.58	1
44	2	CARBON TETRACHLORIDE	331.10	1.79	1
17	36	ETHYL ACETATE	331.70	1.45	1
9	4	CHLOROFORM	331.90	2.60	1
66	4	CHLOROFORM	331.90	0.86	1
11	4	CHLOROFORM	331.90	1.35	1
80	4	CHLOROFORM	331.90	1.66	1
44	36	ETHYL ACETATE	331.90	1.12	1
21	66	BENZENE	332.10	1.63	1
66	72	CYCLOHEXANE	332.95	1.41	1
21	2	CARBON TETRACHLORIDE	333.00	2.76	1
26	2	CARBON TETRACHLORIDE	333.00	4.24	1
66	8	METHANOL	333.15	5.80	11
80	8	METHANOL	333.15	19.00	11
80	9	NITROMETHANE	333.15	22.00	11
80	11	ACETONITRILE	333.15	15.80	11
66	20	PROPIONITRILE	333.15	1.48	11
80	20	PROPIONITRILE	333.15	7.40	11
66	21	ACETONE	333.15	1.60	11
80	21	ACETONE	333.15	5.10	11
8	21	ACETONE	333.15	1.73	21
80	44	PYRIDINE	333.15	4.80	11
66	44	PYRIDINE	333.15	1.20	11
66	64	NITROBENZENE	333.15	1.10	11
80	64	NITROBENZENE	333.15	5.10	11
80	68	ANILINE	333.15	14.00	11
66	68	ANILINE	333.15	2.00	11
66	11	ACETONITRILE	333.20	2.66	14
18	32	2-BUTANONE	333.30	1.00	1
8	32	2-BUTANONE	333.30	2.09	1
9	32	2-BUTANONE	333.30	1.23	1
14	32	2-BUTANONE	333.30	0.79	1
94	32	2-BUTANONE	333.30	3.35	1

SLT	SLV		TEMP	GAMMA INFINITY	REF
19	32	2-BUTANONE	333.30	1.99	1
36	32	2-BUTANONE	333.30	1.10	1
11	32	2-BUTANONE	333.30	1.25	1
19	36	ETHYL ACETATE	333.50	2.42	1
32	36	ETHYL ACETATE	333.50	1.08	1
34	36	ETHYL ACETATE	333.50	1.06	1
91	36	ETHYL ACETATE	333.50	1.18	1
26	72	CYCLOHEXANE	333.70	8.15	1
14	72	CYCLOHEXANE	334.18	2.52	1
44	11	ACETONITRILE	334.60	1.81	1
80	14	1,2-DICHLOROETHANE	334.60	3.59	1
87	2	CARBON TETRACHLORIDE	335.20	0.79	1
98	66	BENZENE	335.43	1.71	1
98	19	ETHANOL	335.52	10.90	1
21	19	ETHANOL	335.79	2.03	1
65	19	ETHANOL	335.80	5.10	1
44	19	ETHANOL	336.40	0.96	1
72	20	PROPIONITRILE	336.70	6.00	1
87	66	BENZENE	336.70	1.24	1
6	34	TETRAHYDROFURAN	336.90	0.50	1
4	37	DIOXANE	337.00	0.50	1
94	14	1,2-DICHLOROETHANE	337.20	3.00	1
21	14	1,2-DICHLOROETHANE	337.20	0.78	1
32	14	1,2-DICHLOROETHANE	337.20	0.77	1
2	14	1,2-DICHLOROETHANE	337.20	1.65	1
66	14	1,2-DICHLOROETHANE	337.20	1.06	1
16	14	1,2-DICHLOROETHANE	337.20	1.41	1
98	14	1,2-DICHLOROETHANE	337.20	3.86	1
8	14	1,2-DICHLOROETHANE	337.20	6.93	1
19	14	1,2-DICHLOROETHANE	337.20	7.20	1
72	34	TETRAHYDROFURAN	337.30	1.59	1
4	34	TETRAHYDROFURAN	337.30	0.37	1
44	20	PROPIONITRILE	338.00	1.39	1
42	11	ACETONITRILE	338.20	12.40	14
91	31	N-PROPANOL	338.20	3.62	17
14	31	N-PROPANOL	338.20	2.97	17
9	2	CARBON TETRACHLORIDE	340.20	9.10	1
32	2	CARBON TETRACHLORIDE	340.20	2.02	1
26	2	CARBON TETRACHLORIDE	340.20	4.10	1
11	2	CARBON TETRACHLORIDE	340.20	8.70	1
14	72	CYCLOHEXANE	340.39	2.44	1
39	72	CYCLOHEXANE	340.69	1.46	1
72	2	CARBON TETRACHLORIDE	341.20	1.09	1
87	32	2-BUTANONE	341.30	2.21	1
44	32	2-BUTANONE	342.20	1.13	1
19	66	BENZENE	342.42	7.90	1
87	36	ETHYL ACETATE	342.70	1.84	1
21	39	N-BUTYL CHLORIDE	343.20	1.42	1

SLT	SLV	SOLVENT	TEMP	GAMMA INFINITY	REF
10	10	SOLVENT			
44	32	2-BUTANONE	343.30	1.14	1
108	14	1,2-DICHLOROETHANE	343.50	3.43	1
11	14	1,2-DICHLOROETHANE	343.90	1.45	1
20	14	1,2-DICHLOROETHANE	343.90	1.11	1
9	14	1,2-DICHLOROETHANE	343.90	1.73	1
17	36	ETHYL ACETATE	343.90	1.41	1
27	19	ETHANOL	344.60	5.46	1
21	2	CARBON TETRACHLORIDE	345.15	2.58	1
14	72	CYCLOHEXANE	345.70	2.36	1
26	72	CYCLOHEXANE	346.10	7.40	1
32	2	CARBON TETRACHLORIDE	346.30	1.98	1
11	2	CARBON TETRACHLORIDE	346.30	8.10	1
26	2	CARBON TETRACHLORIDE	346.30	3.96	1
66	19	ETHANOL	346.39	4.40	1
72	2	CARBON TETRACHLORIDE	346.50	1.10	1
21	2	CARBON TETRACHLORIDE	346.80	2.59	1
21	2	CARBON TETRACHLORIDE	346.97	2.52	1
87	2	CARBON TETRACHLORIDE	347.10	0.81	1
14	36	ETHYL ACETATE	347.80	0.85	1
11	36	ETHYL ACETATE	347.80	1.51	1
32	36	ETHYL ACETATE	347.80	1.04	1
98	19	ETHANOL	347.81	10.30	1
65	19	ETHANOL	347.96	4.90	1
72	70	CYCLOHEXANONE	348.20	2.24	4
21	19	ETHANOL	348.26	1.92	1
34	36	ETHYL ACETATE	348.30	1.03	1
19	36	ETHYL ACETATE	348.30	2.33	1
91	36	ETHYL ACETATE	348.30	1.14	1
44	39	N-BUTYL CHLORIDE	348.30	1.35	1
80	36	ETHYL ACETATE	348.40	2.41	1
36	32	2-BUTANONE	348.60	1.10	1
19	32	2-BUTANONE	348.60	1.74	1
94	32	2-BUTANONE	348.60	3.08	1
44	2	CARBON TETRACHLORIDE	348.90	1.72	1
9	36	ETHYL ACETATE	348.90	1.42	2
19	66	BENZENE	348.97	7.60	1
87	39	N-BUTYL CHLORIDE	349.00	1.11	2
98	2	CARBON TETRACHLORIDE	349.10	1.15	1
9	2	CARBON TETRACHLORIDE	349.10	8.40	1
66	2	CARBON TETRACHLORIDE	349.10	1.10	1
32	19	ETHANOL	349.15	1.72	4
20	36	ETHYL ACETATE	349.20	1.29	1
4	36	ETHYL ACETATE	349.20	0.52	1
44	39	N-BUTYL CHLORIDE	349.30	1.38	1
98	66	BENZENE	349.38	1.59	1
91	19	ETHANOL	349.44	5.14	1
21	66	BENZENE	349.70	1.62	1
72	2	CARBON TETRACHLORIDE	349.80	1.10	1

SLT	SLV		TEMP	GAMMA INFINITY	REF
	ID	SOLVENT			
44	36	ETHYL ACETATE	349.80	1.14	1
14	32	2-BUTANONE	350.20	0.82	1
9	32	2-BUTANONE	350.20	1.20	1
8	36	ETHYL ACETATE	350.30	2.65	1
21	66	BENZENE	350.50	1.60	1
44	19	ETHANOL	350.60	0.94	1
72	66	BENZENE	350.60	1.45	1
39	72	CYCLOHEXANE	350.79	1.43	1
21	39	N-BUTYL CHLORIDE	350.80	1.40	1
32	72	CYCLOHEXANE	350.80	3.70	1
66	72	CYCLOHEXANE	350.80	1.38	1
27	19	ETHANOL	350.90	5.19	1
80	19	ETHANOL	350.90	8.10	1
44	66	BENZENE	351.10	1.22	1
14	72	CYCLOHEXANE	351.17	2.29	1
66	19	ETHANOL	351.40	4.34	1
26	72	CYCLOHEXANE	351.70	6.87	1
87	32	2-BUTANONE	352.00	2.12	1
118	66	BENZENE	352.30	1.14	1
66	72	CYCLOHEXANE	352.31	1.35	1
87	66	BENZENE	352.40	1.21	1
44	11	ACETONITRILE	352.60	1.75	1
2	11	ACETONITRILE	352.62	4.90	1
118	66	BENZENE	352.80	1.11	1
65	24	1-NITROPROPANE	353.54	1.35	32
24	65	CHLOROBENZENE	353.63	1.70	1
2	72	CYCLOHEXANE	353.80	1.07	1
87	14	1,2-DICHLOROETHANE	354.20	1.82	1
44	14	1,2-DICHLOROETHANE	354.30	0.89	1
2	14	1,2-DICHLOROETHANE	354.30	1.55	1
80	14	1,2-DICHLOROETHANE	354.70	3.01	1
32	14	1,2-DICHLOROETHANE	354.70	0.78	1
94	14	1,2-DICHLOROETHANE	354.70	2.61	1
21	14	1,2-DICHLOROETHANE	354.70	0.78	1
86	14	1,2-DICHLOROETHANE	355.20	1.04	1
8	14	1,2-DICHLOROETHANE	355.20	5.50	1
98	14	1,2-DICHLOROETHANE	355.30	3.10	1
16	14	1,2-DICHLOROETHANE	355.30	1.39	1
20	14	1,2-DICHLOROETHANE	355.30	1.11	1
11	14	1,2-DICHLOROETHANE	355.30	1.43	1
9	14	1,2-DICHLOROETHANE	355.30	1.63	1
72	20	PROPIONITRILE	356.30	5.22	1
66	9	NITROMETHANE	358.90	3.06	1
4	37	DIOXANE	360.33	0.57	1
4	37	DIOXANE	370.04	0.61	1
66	9	NITROMETHANE	371.50	2.65	1
68	8	METHANOL	373.15	4.70	11
80	8	METHANOL	373.15	13.50	11

SLT	SLV	SOLVENT	TEMP	GAMMA INFINITY	REF
80	9	NITROMETHANE	373.15	12.00	11
80	11	ACETONITRILE	373.15	10.80	11
66	11	ACETONITRILE	373.15	2.40	11
80	20	PROPIONITRILE	373.15	5.50	11
66	20	PROPIONITRILE	373.15	1.40	11
80	21	ACETONE	373.15	4.50	11
66	21	ACETONE	373.15	1.50	11
66	44	PYRIDINE	373.15	1.20	11
80	44	PYRIDINE	373.15	3.80	11
66	64	NITROBENZENE	373.15	1.00	11
80	64	NITROBENZENE	373.15	3.70	11
80	68	ANILINE	373.15	8.00	11
66	68	ANILINE	373.15	1.80	11
91	70	CYCLOHEXANONE	428.80	0.98	4
61	60	N-PENTYL BROMIDE	223.20	2.00	3 *
60	61	N-PENTANE	233.20	2.55	3 *
21	61	N-PENTANE	238.20	16.80	3 *
80	42	N-BUTANE	253.00	0.95	3 *
61	21	ACETONE	258.20	8.95	3 *
21	61	N-PENTANE	258.20	11.50	3 *
80	21	ACETONE	268.20	9.86	3 *
61	20	PROPIONITRILE	273.15	10.50	13 *
50	20	PROPIONITRILE	273.15	5.27	13 *
61	21	ACETONE	273.15	6.79	13 *
50	21	ACETONE	273.15	3.69	13 *
61	32	2-BUTANONE	273.15	4.15	13 *
50	32	2-BUTANONE	273.15	2.40	13 *
66	2	CARBON TETRACHLORIDE	273.20	1.14	3 *
50	11	ACETONITRILE	273.20	12.00	13 *
21	68	ANILINE	277.40	0.71	15 *
98	25	DIMETHYL FORMAMIDE	278.30	28.70	3 *
72	66	BENZENE	281.20	1.96	27 *
66	72	CYCLOHEXANE	281.20	1.79	27 *
87	31	N-PROPANOL	283.20	0.93	3 *
74	66	BENZENE	283.20	1.76	3 *
85	66	BENZENE	283.20	2.62	3 *
66	71	4-METHYL 1-PENTENE	283.20	1.49	3 *
72	66	BENZENE	287.20	1.89	27 *
66	72	CYCLOHEXANE	287.20	1.75	27 *
66	11	ACETONITRILE	293.15	3.19	3 *
66	43	N-BUTANOL	293.15	2.95	29 *
8	2	CARBON TETRACHLORIDE	293.20	45.40	3 *
31	2	CARBON TETRACHLORIDE	293.20	22.50	3 *
19	2	CARBON TETRACHLORIDE	293.20	36.20	3 *
21	8	METHANOL	293.20	2.27	3 *
23	8	METHANOL	293.20	3.33	3 *
68	8	METHANOL	293.20	3.05	15 *
19	11	ACETONITRILE	293.20	4.32	12 *

SLT	SLV		TEMP	GAMMA INFINITY	REF
91	11	ACETONITRILE	293.20	4.50	12 *
98	11	ACETONITRILE	293.20	46.00	3 *
68	11	ACETONITRILE	293.20	1.18	15 *
72	14	1,2-DICHLOROETHANE	293.20	4.50	3 *
21	17	ETHYL IODIDE	293.20	2.84	3 *
37	19	ETHANOL	293.20	3.41	3 *
2	19	ETHANOL	293.20	5.18	3 *
72	19	ETHANOL	293.20	10.25	3 *
11	19	ETHANOL	293.20	4.33	12 *
1	19	ETHANOL	293.20	6.47	3 *
80	21	ACETONE	293.20	6.96	3 *
17	21	ACETONE	293.20	2.84	3 *
4	21	ACETONE	293.20	0.40	3 *
8	23	METHYL ACETATE	293.20	3.15	3 *
2	31	N-PROPANOL	293.20	4.14	3 *
8	37	DIOXANE	293.20	2.60	3 *
1	37	DIOXANE	293.20	2.39	3 *
80	42	N-BUTANE	293.20	0.86	3 *
72	44	PYRIDINE	293.20	4.57	3 *
61	60	N-PENTYL BROMIDE	293.20	1.56	3 *
60	61	N-PENTANE	293.20	1.78	3 *
102	65	CHLOROBENZENE	293.20	0.99	3 *
68	65	CHLOROBENZENE	293.20	3.34	15 *
14	66	BENZENE	293.20	1.04	3 *
11	66	BENZENE	293.20	3.31	3 *
72	66	BENZENE	293.20	1.83	27 *
28	68	ANILINE	293.20	2.96	15 *
65	68	ANILINE	293.20	2.60	15 *
80	68	ANILINE	293.20	23.20	3 *
8	68	ANILINE	293.20	2.39	15 *
11	68	ANILINE	293.20	1.00	15 *
91	72	CYCLOHEXANE	293.20	1.67	3 *
66	72	CYCLOHEXANE	293.20	1.69	27 *
19	72	CYCLOHEXANE	293.20	49.10	3 *
14	72	CYCLOHEXANE	293.20	3.87	3 *
44	72	CYCLOHEXANE	293.20	6.48	3 *
80	64	NITROBENZENE	294.20	8.10	3 *
24	2	CARBON TETRACHLORIDE	298.15	4.48	8 *
21	8	METHANOL	298.15	2.03	19 *
34	8	METHANOL	298.15	2.40	25 *
36	8	METHANOL	298.15	3.50	25 *
32	8	METHANOL	298.15	2.36	19 *
98	19	ETHANOL	298.15	16.00	19 *
61	19	ETHANOL	298.15	9.00	19 *
72	19	ETHANOL	298.15	9.50	19 *
80	19	ETHANOL	298.15	12.00	19 *
36	19	ETHANOL	298.15	3.20	19 *
50	20	PROPIONITRILE	298.15	4.48	13 *

SLT	SLV	SOLVENT	TEMP	GAMMA INFINITY	REF
61	20	PROPIONITRILE	298.15	8.28	13 *
61	21	ACETONE	298.15	5.28	13 *
50	21	ACETONE	298.15	3.16	13 *
61	32	2-BUTANONE	298.15	3.42	13 *
50	32	2-BUTANONE	298.15	2.11	13 *
98	32	2-BUTANONE	298.15	4.45	19 *
91	32	2-BUTANONE	298.15	1.50	19 *
66	32	2-BUTANONE	298.15	1.12	19 *
8	34	TETRAHYDROFURAN	298.15	2.60	25 *
8	36	ETHYL ACETATE	298.15	4.30	25 *
61	44	PYRIDINE	298.15	6.24	13 *
50	44	PYRIDINE	298.15	3.77	13 *
66	1	CARBON DISULFIDE	298.20	1.56	3 *
72	1	CARBON DISULFIDE	298.20	1.59	3 *
47	1	CARBON DISULFIDE	298.20	1.54	3 *
47	2	CARBON TETRACHLORIDE	298.20	1.06	3 *
80	2	CARBON TETRACHLORIDE	298.20	1.46	3 *
47	4	CHLOROFORM	298.20	1.53	3 *
33	8	METHANOL	298.20	3.85	3 *
97	8	METHANOL	298.20	5.59	19 *
55	8	METHANOL	298.20	3.27	19 *
66	9	NITROMETHANE	298.20	3.84	3 *
50	11	ACETONITRILE	298.20	9.45	13 *
61	11	ACETONITRILE	298.20	20.40	13 *
66	16	NITROETHANE	298.20	1.80	3 *
33	19	ETHANOL	298.20	3.19	3 *
42	19	ETHANOL	298.20	7.60	19 *
123	19	ETHANOL	298.20	22.50	19 *
107	19	ETHANOL	298.20	13.50	19 *
136	19	ETHANOL	298.20	155.00	19 *
102	19	ETHANOL	298.20	1.30	19 *
133	19	ETHANOL	298.20	77.00	19 *
126	19	ETHANOL	298.20	28.00	19 *
91	20	PROPIONITRILE	298.20	2.22	3 *
72	21	ACETONE	298.20	6.68	3 *
4	21	ACETONE	298.20	0.43	3 *
54	21	ACETONE	298.20	2.67	3 *
61	21	ACETONE	298.20	5.75	3 *
98	25	DIMETHYL FORMAMIDE	298.20	21.50	3 *
121	32	2-BUTANONE	298.20	4.40	19 *
72	32	2-BUTANONE	298.20	3.40	19 *
126	32	2-BUTANONE	298.20	6.10	19 *
107	32	2-BUTANONE	298.20	4.90	19 *
120	32	2-BUTANONE	298.20	2.25	19 *
123	32	2-BUTANONE	298.20	6.60	19 *
102	32	2-BUTANONE	298.20	1.77	19 *
8	33	METHYL PROPIONATE	298.20	4.71	3 *
2	34	TETRAHYDROFURAN	298.20	0.75	3 *

SLT	SLV	SOLVENT	TEMP	GAMMA INFINITY	REF
79	43	N-BUTANOL	298.20	3.00	3 *
32	43	N-BUTANOL	298.20	1.98	19 *
97	43	N-BUTANOL	298.20	2.67	3 *
87	43	N-BUTANOL	298.20	0.84	3 *
2	47	CYCLOPENTANE	298.20	1.05	3 *
4	47	CYCLOPENTANE	298.20	1.53	3 *
66	47	CYCLOPENTANE	298.20	1.60	3 *
66	47	CYCLOPENTANE	298.20	1.67	26 *
81	47	CYCLOPENTANE	298.20	1.15	3 *
1	47	CYCLOPENTANE	298.20	1.39	3 *
80	61	N-PENTANE	298.20	0.95	3 *
66	61	N-PENTANE	298.20	1.97	26 *
21	61	N-PENTANE	298.20	7.10	3 *
83	63	1-PENTANOL	298.20	3.38	3 *
85	63	1-PENTANOL	298.20	3.45	3 *
81	63	1-PENTANOL	298.20	3.35	3 *
80	63	1-PENTANOL	298.20	4.26	3 *
66	64	NITROBENZENE	298.20	1.36	3 *
94	66	BENZENE	298.20	1.80	26 *
69	66	BENZENE	298.20	1.30	3 *
109	66	BENZENE	298.20	2.03	26 *
61	66	BENZENE	298.20	2.09	26 *
80	66	BENZENE	298.20	2.13	3 *
47	66	BENZENE	298.20	1.54	3 *
73	66	BENZENE	298.20	1.59	3 *
16	66	BENZENE	298.20	2.14	3 *
98	66	BENZENE	298.20	2.15	26 *
72	66	BENZENE	298.20	1.66	3 *
75	66	BENZENE	298.20	1.72	26 *
1	66	BENZENE	298.20	1.37	3 *
126	67	PHENOL	298.20	31.00	19 *
66	67	PHENOL	298.20	2.90	19 *
123	67	PHENOL	298.20	22.00	19 *
102	67	PHENOL	298.20	5.30	19 *
107	67	PHENOL	298.20	17.00	19 *
61	67	PHENOL	298.20	15.00	19 *
91	67	PHENOL	298.20	3.90	19 *
98	67	PHENOL	298.20	20.00	19 *
136	67	PHENOL	298.20	105.00	19 *
72	67	PHENOL	298.20	11.80	19 *
121	67	PHENOL	298.20	19.00	19 *
133	67	PHENOL	298.20	66.50	19 *
66	69	CYCLOHEXENE	298.20	1.25	3 *
1	72	CYCLOHEXANE	298.20	1.28	3 *
91	72	CYCLOHEXANE	298.20	1.73	26 *
103	72	CYCLOHEXANE	298.20	1.72	3 *
21	72	CYCLOHEXANE	298.20	8.81	3 *
66	73	1-HEXENE	298.20	1.45	3 *

SLT	SLV		TEMP	GAMMA INFINITY	REF	
91	75	METHYL CYCLOPENTANE	298.20	1.59	26	*
66	75	METHYL CYCLOPENTANE	298.20	1.74	26	*
32	62	ISOPENTANE	301.00	4.98	3	*
25	62	ISOPENTANE	301.00	33.30	3	*
32	50	1-PENTENE	303.10	2.84	3	*
21	50	1-PENTENE	303.10	4.15	3	*
11	50	1-PENTENE	303.10	13.90	3	*
34	2	CARBON TETRACHLORIDE	303.15	0.83	10	*
37	4	CHLOROFORM	303.15	0.21	10	*
34	4	CHLOROFORM	303.15	0.21	10	*
44	4	CHLOROFORM	303.15	0.20	10	*
44	6	DICHLOROMETHANE	303.15	0.32	10	*
37	6	DICHLOROMETHANE	303.15	0.37	10	*
21	6	DICHLOROMETHANE	303.15	0.46	10	*
34	6	DICHLOROMETHANE	303.15	0.36	10	*
6	21	ACETONE	303.15	0.56	10	*
44	21	ACETONE	303.15	1.21	10	*
37	25	DIMETHYL FORMAMIDE	303.15	1.32	3	*
98	31	N-PROPANOL	303.15	7.80	48	*
4	34	TETRAHYDROFURAN	303.15	0.27	10	*
2	34	TETRAHYDROFURAN	303.15	0.87	10	*
6	34	TETRAHYDROFURAN	303.15	0.40	10	*
4	37	DIOXANE	303.15	0.47	10	*
6	37	DIOXANE	303.15	0.53	10	*
4	44	PYRIDINE	303.15	0.45	10	*
6	44	PYRIDINE	303.15	0.58	10	*
21	44	PYRIDINE	303.15	1.23	10	*
103	2	CARBON TETRACHLORIDE	303.20	0.88	3	*
11	8	METHANOL	303.20	2.44	3	*
8	9	NITROMETHANE	303.20	4.83	3	*
19	11	ACETONITRILE	303.20	3.09	3	*
8	11	ACETONITRILE	303.20	3.03	3	*
104	14	1,2-DICHLOROETHANE	303.20	1.22	3	*
103	14	1,2-DICHLOROETHANE	303.20	1.31	3	*
98	17	ETHYL IODIDE	303.20	2.32	3	*
19	18	ETHYL BROMIDE	303.20	14.10	3	*
17	19	ETHANOL	303.20	4.94	3	*
18	19	ETHANOL	303.20	4.02	3	*
94	19	ETHANOL	303.20	11.20	3	*
4	21	ACETONE	303.20	0.46	3	*
8	21	ACETONE	303.20	1.94	3	*
66	31	N-PROPANOL	303.20	3.67	3	*
2	37	DIOXANE	303.20	1.17	3	*
25	37	DIOXANE	303.20	1.78	3	*
61	43	N-BUTANOL	303.20	4.14	3	*
91	44	PYRIDINE	303.20	1.36	3	*
61	63	1-PENTANOL	303.20	3.64	3	*
91	65	CHLOROBENZENE	303.20	0.96	3	*

SLT	SLV		TEMP	GAMMA INFINITY	REF	
ID	ID	SOLVENT				
106	66	BENZENE	303.20	1.63	3	*
31	66	BENZENE	303.20	13.20	3	*
66	67	PHENOL	303.20	2.20	13	*
104	72	CYCLOHEXANE	303.20	1.93	3	*
102	72	CYCLOHEXANE	303.20	1.67	3	*
91	73	1-HEXENE	303.20	1.30	3	*
66	74	2-METHYL-1-PENTENE	303.20	1.39	3	*
19	21	ACETONE	305.20	1.98	3	*
133	72	CYCLOHEXANE	305.20	0.65	3	*
128	72	CYCLOHEXANE	305.30	0.87	3	*
8	46	ISOPRENE	307.20	33.20	3	*
21	46	ISOPRENE	307.20	2.30	3	*
11	46	ISOPRENE	307.20	5.70	3	*
11	46	ISOPRENE	307.20	5.50	3	*
25	46	ISOPRENE	307.20	8.50	3	*
9	46	ISOPRENE	307.20	6.70	3	*
80	4	CHLOROFORM	308.10	1.83	53	*
66	8	METHANOL	308.10	7.18	53	*
8	66	BENZENE	308.10	17.30	3	*
61	11	ACETONITRILE	308.15	17.30	13	*
50	11	ACETONITRILE	308.15	8.68	13	*
61	20	PROPIONITRILE	308.15	7.61	13	*
50	20	PROPIONITRILE	308.15	4.25	13	*
50	21	ACETONE	308.15	2.94	13	*
61	21	ACETONE	308.15	4.81	13	*
50	32	2-BUTANONE	308.15	2.02	13	*
61	32	2-BUTANONE	308.15	3.18	13	*
91	2	CARBON TETRACHLORIDE	308.20	1.08	3	*
19	4	CHLOROFORM	308.20	4.90	50	*
4	8	METHANOL	308.20	2.60	3	*
37	8	METHANOL	308.20	3.16	3	*
66	10	METHYL IODIDE	308.20	1.16	3	*
87	19	ETHANOL	308.20	1.30	3	*
4	19	ETHANOL	308.20	1.60	50	*
4	21	ACETONE	308.20	0.47	3	*
72	21	ACETONE	308.20	5.73	3	*
80	21	ACETONE	308.20	6.15	3	*
66	21	ACETONE	308.20	1.52	3	*
8	37	DIOXANE	308.20	2.53	3	*
80	64	NITROBENZENE	308.20	7.90	3	*
10	66	BENZENE	308.20	1.12	3	*
21	72	CYCLOHEXANE	308.20	6.99	3	*
19	72	CYCLOHEXANE	308.20	39.10	3	*
21	1	CARBON DISULFIDE	308.30	7.40	5	*
1	21	ACETONE	308.30	3.98	3	*
21	61	N-PENTANE	309.20	6.17	3	*
8	61	N-PENTANE	309.20	53.10	3	*
75	61	N-PENTANE	309.20	1.08	3	*

SLT	SLV		TEMP	GAMMA INFINITY	REF
10	10	SOLVENT			
94	61	N-PENTANE	309.20	1.08	3 *
72	61	N-PENTANE	309.20	1.11	3 *
32	48	I-PENTENE	309.80	2.84	3 *
9	48	I-PENTENE	309.80	17.10	3 *
66	18	ETHYL BROMIDE	311.50	0.96	3 *
87	19	ETHANOL	311.60	1.10	40 *
11	48	I-PENTENE	311.70	13.70	3 *
61	6	DICHLOROMETHANE	313.00	2.35	3 *
8	6	DICHLOROMETHANE	313.00	7.91	3 *
19	6	DICHLOROMETHANE	313.00	4.27	3 *
19	11	ACETONITRILE	313.15	3.70	16 *
19	14	1,2-DICHLOROETHANE	313.15	9.00	18 *
14	19	ETHANOL	313.15	4.40	18 *
11	19	ETHANOL	313.15	3.50	16 *
37	25	DIMETHYL FORMAMIDE	313.15	1.31	3 *
14	8	METHANOL	313.20	4.75	3 *
36	8	METHANOL	313.20	3.20	19 *
66	8	METHANOL	313.20	7.24	3 *
36	11	ACETONITRILE	313.20	1.53	12 *
98	11	ACETONITRILE	313.20	32.80	3 *
68	19	ETHANOL	313.20	3.18	47 *
14	19	ETHANOL	313.20	4.52	3 *
11	19	ETHANOL	313.20	3.68	3 *
36	19	ETHANOL	313.20	2.82	3 *
21	19	ETHANOL	313.20	2.16	3 *
8	19	ETHANOL	313.20	0.98	3 *
61	21	ACETONE	313.20	4.40	19 *
4	21	ACETONE	313.20	0.49	3 *
128	21	ACETONE	313.20	11.80	3 *
8	23	METHYL ACETATE	313.20	2.76	3 *
87	31	N-PROPANOL	313.20	1.26	3 *
19	36	ETHYL ACETATE	313.20	2.84	3 *
11	36	ETHYL ACETATE	313.20	1.53	12 *
108	44	PYRIDINE	313.20	8.00	3 *
60	50	1-PENTENE	313.20	18.10	15 *
66	61	N-PENTANE	313.20	1.79	3 *
133	66	BENZENE	313.20	1.13	3 *
50	68	ANILINE	313.20	8.83	15 *
19	68	ANILINE	313.20	2.67	47 *
44	72	CYCLOHEXANE	313.20	5.28	3 *
106	72	CYCLOHEXANE	313.20	1.09	3 *
2	72	CYCLOHEXANE	313.20	1.11	3 *
66	72	CYCLOHEXANE	313.20	1.52	3 *
91	72	CYCLOHEXANE	313.20	1.53	3 *
68	21	ACETONE	313.40	0.74	15 *
21	68	ANILINE	313.40	0.87	15 *
80	4	CHLOROFORM	318.10	1.79	53 *
11	2	CARBON TETRACHLORIDE	318.15	9.80	8 *

SLT	SLV	SOLVENT	TEMP	GAMMA INFINITY	REF
21	2	CARBON TETRACHLORIDE	318.15	3.00	8 *
9	2	CARBON TETRACHLORIDE	318.15	10.60	8 *
2	9	NITROMETHANE	318.15	7.45	8 *
21	9	NITROMETHANE	318.15	0.94	8 *
2	11	ACETONITRILE	318.15	5.90	8 *
61	11	ACETONITRILE	318.15	15.40	13 *
66	19	ETHANOL	318.15	4.45	8 *
61	20	PROPIONITRILE	318.15	7.00	13 *
50	20	PROPIONITRILE	318.15	4.00	13 *
2	21	ACETONE	318.15	2.15	8 *
66	21	ACETONE	318.15	1.52	8 *
61	21	ACETONE	318.15	4.41	13 *
50	21	ACETONE	318.15	2.80	13 *
9	21	ACETONE	318.15	0.96	8 *
50	32	2-BUTANONE	318.15	1.92	13 *
61	32	2-BUTANONE	318.15	2.99	13 *
19	66	BENZENE	318.15	10.60	8 *
43	66	BENZENE	318.15	9.20	29 *
21	66	BENZENE	318.15	1.65	8 *
11	66	BENZENE	318.15	3.20	8 *
108	2	CARBON TETRACHLORIDE	318.20	1.40	3 *
23	8	METHANOL	318.20	3.00	19 *
22	8	METHANOL	318.20	3.07	3 *
66	9	NITROMETHANE	318.20	3.39	3 *
66	11	ACETONITRILE	318.20	2.74	3 *
91	11	ACETONITRILE	318.20	3.63	3 *
21	11	ACETONITRILE	318.20	1.03	3 *
91	16	NITROETHANE	318.20	2.02	3 *
22	19	ETHANOL	318.20	3.22	3 *
72	21	ACETONE	318.20	4.67	3 *
4	21	ACETONE	318.20	0.49	3 *
80	21	ACETONE	318.20	5.53	3 *
11	21	ACETONE	318.20	1.04	3 *
8	22	ETHYL FORMATE	318.20	3.54	3 *
19	22	ETHYL FORMATE	318.20	3.55	3 *
31	23	METHYL ACETATE	318.20	2.79	3 *
23	31	N-PROPANOL	318.20	3.59	3 *
8	34	TETRAHYDROFURAN	318.20	2.36	3 *
72	44	PYRIDINE	318.20	3.51	3 *
66	47	CYCLOPENTANE	318.20	1.48	3 *
61	66	BENZENE	318.20	1.82	3 *
9	66	BENZENE	318.20	3.20	3 *
21	72	CYCLOHEXANE	318.20	5.63	3 *
11	66	BENZENE	318.30	2.94	3 *
8	1	CARBON DISULFIDE	319.30	45.00	7 *
8	28	N-PROPYL CHLORIDE	319.60	11.50	3 *
66	47	CYCLOPENTANE	322.40	1.39	3 *
136	72	CYCLOHEXANE	322.70	0.50	3 *

SLT	SLV	SOLVENT	TEMP	GAMMA INFINITY	REF
66	4	CHLOROFORM	323.10	0.81	28 *
98	43	N-BUTANOL	323.10	4.94	56 *
4	66	BENZENE	323.10	0.81	28 *
8	32	2-BUTANONE	323.14	2.10	23 *
21	4	CHLOROFORM	323.15	0.44	8 *
21	8	METHANOL	323.15	2.06	8 *
32	8	METHANOL	323.15	2.24	3 *
61	19	ETHANOL	323.15	8.10	19 *
98	19	ETHANOL	323.15	13.00	19 *
4	21	ACETONE	323.15	0.54	8 *
8	21	ACETONE	323.15	1.78	8 *
104	2	CARBON TETRACHLORIDE	323.20	0.86	3 *
98	4	CHLOROFORM	323.20	1.70	3 *
19	14	1,2-DICHLOROETHANE	323.20	7.82	3 *
133	19	ETHANOL	323.20	46.00	19 *
102	19	ETHANOL	323.20	9.00	19 *
123	19	ETHANOL	323.20	18.00	19 *
136	19	ETHANOL	323.20	70.00	19 *
91	19	ETHANOL	323.20	5.42	3 *
107	19	ETHANOL	323.20	12.00	19 *
126	19	ETHANOL	323.20	20.20	19 *
42	19	ETHANOL	323.20	6.90	19 *
4	21	ACETONE	323.20	0.51	3 *
98	21	ACETONE	323.20	6.72	3 *
31	22	ETHYL FORMATE	323.20	3.18	3 *
22	31	N-PROPANOL	323.20	2.90	3 *
8	31	N-PROPANOL	323.20	1.19	3 *
102	32	2-BUTANONE	323.20	1.62	19 *
126	32	2-BUTANONE	323.20	4.50	19 *
123	32	2-BUTANONE	323.20	5.10	19 *
2	32	2-BUTANONE	323.20	1.62	3 *
107	32	2-BUTANONE	323.20	4.10	19 *
120	32	2-BUTANONE	323.20	1.98	19 *
66	32	2-BUTANONE	323.20	1.16	3 *
91	32	2-BUTANONE	323.20	1.47	3 *
8	37	DIOXANE	323.20	2.31	3 *
6	37	DIOXANE	323.20	0.46	3 *
98	39	N-BUTYL CHLORIDE	323.20	1.72	3 *
98	41	N-BUTYL BROMIDE	323.20	1.54	3 *
72	43	N-BUTANOL	323.20	3.66	3 *
32	43	N-BUTANOL	323.20	2.01	3 *
91	56	2-PENTANONE	323.20	1.11	3 *
80	63	1-PENTANOL	323.20	3.93	3 *
85	66	BENZENE	323.20	2.02	3 *
106	66	BENZENE	323.20	1.46	3 *
74	66	BENZENE	323.20	1.50	3 *
32	66	BENZENE	323.20	1.30	3 *
19	66	BENZENE	323.20	11.20	3 *

SLT	SLV		TEMP	GAMMA INFINITY	RFF	
	ID	SOLVENT				
71	66	BENZENE	323.20	1.47	3	*
102	67	PHENOL	323.20	3.70	19	*
91	67	PHENOL	323.20	3.30	19	*
61	67	PHENOL	323.20	11.30	19	*
98	67	PHENOL	323.20	15.40	19	*
123	67	PHENOL	323.20	15.50	19	*
66	67	PHENOL	323.20	2.50	19	*
136	67	PHENOL	323.20	72.00	19	*
72	67	PHENOL	323.20	8.70	19	*
126	67	PHENOL	323.20	23.50	19	*
107	67	PHENOL	323.20	12.50	19	*
133	67	PHENOL	323.20	48.00	19	*
66	71	4-METHYL 1-PENTENE	323.20	1.36	3	*
43	72	CYCLOHEXANE	323.20	23.50	3	*
104	72	CYCLOHEXANE	323.20	1.82	3	*
19	72	CYCLOHEXANE	323.20	28.20	3	*
102	72	CYCLOHEXANE	323.20	1.57	3	*
66	74	2-METHYL-1-PENTENE	323.20	1.34	3	*
22	8	METHANOL	324.20	3.00	19	*
80	4	CHLOROFORM	328.10	1.72	53	*
66	8	METHANOL	328.10	6.50	53	*
8	66	BENZENE	328.10	12.10	6	*
21	72	CYCLOHEXANE	328.10	6.07	3	*
19	4	CHLOROFORM	328.20	4.10	50	*
72	8	METHANOL	328.20	17.70	3	*
50	11	ACETONITRILE	328.20	7.97	13	*
4	19	ETHANOL	328.20	1.74	3	*
72	21	ACETONE	328.20	4.16	3	*
80	21	ACETONE	328.20	5.20	3	*
4	21	ACETONE	328.20	0.52	3	*
73	29	N-PROPYL BROMIDE	328.20	1.38	3	*
8	36	ETHYL ACETATE	328.20	2.96	3	*
8	72	CYCLOHEXANE	328.20	31.80	3	*
103	72	CYCLOHEXANE	328.20	1.56	3	*
21	72	CYCLOHEXANE	328.20	5.34	3	*
29	73	1-HEXENE	328.20	1.47	3	*
43	21	ACETONE	328.80	1.76	3	*
14	21	ACETONE	329.20	0.93	3	*
13	21	ACETONE	329.20	0.80	3	*
91	21	ACETONE	329.20	1.55	3	*
2	21	ACETONE	329.40	2.15	3	*
73	21	ACETONE	329.40	3.26	3	*
66	21	ACETONE	329.40	1.40	3	*
61	21	ACETONE	329.40	4.10	3	*
46	21	ACETONE	329.40	1.99	3	*
65	21	ACETONE	329.40	1.28	20	*
81	21	ACETONE	329.40	4.62	3	*
8	21	ACETONE	329.40	1.81	3	*

SLT	SLV	SOLVENT	TEMP	GAMMA INFINITY	REF
36	21	ACETONE	329.40	1.13	3 *
19	21	ACETONE	329.40	1.73	3 *
66	19	ETHANOL	329.70	4.70	3 *
21	8	METHANOL	333.15	1.80	19 *
32	8	METHANOL	333.15	2.15	19 *
11	9	NITROMETHANE	333.15	0.96	8 *
9	11	ACETONITRILE	333.15	1.00	8 *
80	19	ETHANOL	333.15	9.70	19 *
36	19	ETHANOL	333.15	2.55	19 *
37	25	DIMETHYL FORMAMIDE	333.15	1.25	3 *
98	32	2-BUTANONE	333.15	3.39	19 *
32	43	N-BUTANOL	333.15	1.64	19 *
62	53	METHYL ISOPROPYL KETONE	333.15	1.90	3 *
46	53	METHYL ISOPROPYL KETONE	333.15	1.15	3 *
48	53	METHYL ISOPROPYL KETONE	333.15	1.50	3 *
98	66	BENZENE	333.15	1.74	3 *
32	73	1-HEXENE	333.15	2.71	67 *
37	8	METHANOL	333.20	2.80	3 *
14	8	METHANOL	333.20	4.35	3 *
23	8	METHANOL	333.20	2.80	19 *
115	8	METHANOL	333.20	7.20	19 *
35	8	METHANOL	333.20	3.00	19 *
73	12	1,1,1-TRICHLOROETHANE	333.20	1.30	3 *
80	12	1,1,1-TRICHLOROETHANE	333.20	1.40	3 *
73	13	1,1,2-TRICHLOROETHANE	333.20	2.01	3 *
80	13	1,1,2-TRICHLOROETHANE	333.20	2.97	3 *
8	14	1,2-DICHLOROETHANE	333.20	7.41	3 *
80	17	ETHYL IODIDE	333.20	2.11	3 *
23	19	ETHANOL	333.20	1.67	3 *
126	21	ACETONE	333.20	6.90	3 *
128	21	ACETONE	333.20	9.23	3 *
98	21	ACETONE	333.20	4.60	19 *
66	25	DIMETHYL FORMAMIDE	333.20	1.54	3 *
126	32	2-BUTANONE	333.20	3.95	19 *
80	32	2-BUTANONE	333.20	3.25	3 *
73	32	2-BUTANONE	333.20	2.51	3 *
8	37	DIOXANE	333.20	2.11	3 *
25	37	DIOXANE	333.20	1.66	3 *
97	43	N-BUTANOL	333.20	2.09	3 *
53	46	ISOPRENE	333.20	1.32	3 *
53	48	1-PENTENE	333.20	2.24	3 *
53	62	ISOPENTANE	333.20	3.55	3 *
75	66	BENZENE	333.20	1.54	3 *
87	66	BENZENE	333.20	1.22	3 *
12	73	1-HEXENE	333.20	1.23	3 *
13	73	1-HEXENE	333.20	1.79	3 *
80	73	1-HEXENE	333.20	1.04	3 *
87	73	1-HEXENE	333.20	1.01	3 *

SLT	SLV	SOLVENT	TEMP	GAMMA INFINITY	REF
80	4	CHLOROFORM	334.10	1.59	52 *
81	4	CHLOROFORM	334.30	1.71	3 *
8	4	CHLOROFORM	334.30	6.94	43 *
43	4	CHLOROFORM	334.30	2.65	3 *
35	4	CHLOROFORM	334.30	0.35	51 *
32	4	CHLOROFORM	334.30	0.43	3 *
21	4	CHLOROFORM	334.30	0.51	43 *
72	66	BENZENE	335.10	1.52	3 *
87	8	METHANOL	335.20	1.81	3 *
21	73	1-HEXENE	336.60	3.30	66 *
2	73	1-HEXENE	336.60	1.10	3 *
37	73	1-HEXENE	336.60	2.42	3 *
19	8	METHANOL	337.20	1.00	43 *
21	8	METHANOL	337.20	1.83	43 *
66	8	METHANOL	337.20	6.68	43 *
34	8	METHANOL	337.20	2.14	3 *
2	8	METHANOL	337.20	9.30	3 *
4	8	METHANOL	337.20	2.54	43 *
6	8	METHANOL	337.40	2.09	3 *
80	75	METHYL CYCLOPENTANE	337.50	1.04	3 *
87	8	METHANOL	337.75	2.20	41 *
92	8	METHANOL	337.80	9.10	3 *
46	8	METHANOL	337.80	7.74	3 *
66	8	METHANOL	337.80	5.89	54 *
32	8	METHANOL	337.80	2.07	3 *
56	8	METHANOL	337.80	2.50	3 *
4	8	METHANOL	337.80	2.57	3 *
48	8	METHANOL	337.80	10.60	3 *
80	8	METHANOL	337.80	18.90	3 *
50	8	METHANOL	337.80	10.00	3 *
21	8	METHANOL	337.80	1.83	3 *
63	8	METHANOL	337.80	1.38	3 *
36	8	METHANOL	337.80	2.81	3 *
28	8	METHANOL	337.80	5.20	3 *
44	8	METHANOL	337.80	1.06	3 *
98	8	METHANOL	337.80	28.40	3 *
66	8	METHANOL	337.80	6.62	3 *
61	8	METHANOL	337.80	14.80	3 *
65	8	METHANOL	337.80	7.76	3 *
19	8	METHANOL	337.80	1.00	3 *
51	8	METHANOL	337.80	8.73	3 *
45	8	METHANOL	337.80	7.22	3 *
81	8	METHANOL	337.80	18.70	3 *
126	8	METHANOL	337.80	53.20	3 *
55	8	METHANOL	337.80	2.73	3 *
1	8	METHANOL	337.80	12.00	7 *
91	8	METHANOL	337.80	8.32	3 *
9	8	METHANOL	337.80	4.60	3 *

SLT	SLV		TEMP	GAMMA INFINITY	REF
52	8	METHANOL	337.80	13.60	3 *
25	8	METHANOL	337.80	0.77	3 *
23	8	METHANOL	337.80	2.78	3 *
43	8	METHANOL	337.80	1.26	3 *
91	8	METHANOL	337.80	7.70	3 *
1	8	METHANOL	337.80	12.10	3 *
87	19	ETHANOL	338.00	1.60	3 *
72	31	N-PROPANOL	338.15	4.83	31 *
31	72	CYCLOHEXANE	338.15	15.19	31 *
19	2	CARBON TETRACHLORIDE	338.20	10.20	3 *
91	2	CARBON TETRACHLORIDE	338.20	1.03	3 *
68	8	METHANOL	338.20	2.77	15 *
72	19	ETHANOL	338.20	8.10	3 *
2	19	ETHANOL	338.20	4.61	3 *
80	55	3-PENTANONE	338.20	2.04	3 *
98	55	3-PENTANONE	338.20	2.35	3 *
80	65	CHLOROBENZENE	338.20	1.95	3 *
8	68	ANILINE	338.20	2.20	15 *
80	68	ANILINE	338.20	12.10	3 *
108	72	CYCLOHEXANE	338.20	1.08	3 *
31	57	N-PROPYL ACETATE	338.90	2.17	3 *
43	34	TETRAHYDROFURAN	339.00	1.16	3 *
68	66	BENZENE	343.10	2.37	3 *
72	68	ANILINE	343.10	8.09	30 *
66	68	ANILINE	343.10	1.92	30 *
68	72	CYCLOHEXANE	343.10	12.30	30 *
61	19	ETHANOL	343.15	7.45	19 *
72	19	ETHANOL	343.15	6.80	19 *
98	19	ETHANOL	343.15	11.80	19 *
91	32	2-BUTANONE	343.15	1.40	19 *
19	11	ACETONITRILE	343.20	2.75	12 *
91	11	ACETONITRILE	343.20	3.65	12 *
68	11	ACETONITRILE	343.20	1.21	15 *
133	19	ETHANOL	343.20	33.50	19 *
42	19	ETHANOL	343.20	6.70	19 *
136	19	ETHANOL	343.20	52.00	19 *
11	19	ETHANOL	343.20	3.15	12 *
123	19	ETHANOL	343.20	16.00	19 *
126	19	ETHANOL	343.20	17.50	19 *
107	19	ETHANOL	343.20	10.70	19 *
102	19	ETHANOL	343.20	8.30	19 *
126	32	2-BUTANONE	343.20	3.70	19 *
120	32	2-BUTANONE	343.20	1.85	19 *
91	63	1-PENTANOL	343.20	3.09	3 *
91	65	CHLOROBENZENE	343.20	1.00	3 *
68	65	CHLOROBENZENE	343.20	2.47	15 *
64	66	BENZENE	343.20	1.48	3 *
107	67	PHENOL	343.20	10.00	19 *

SLT	SLV		TEMP	GAMMA INFINITY	REF
	ID	SOLVENT			
91	67	PHENOL	343.20	2.92	19 *
126	67	PHENOL	343.20	19.50	19 *
123	67	PHENOL	343.20	12.50	19 *
98	67	PHENOL	343.20	12.50	19 *
120	67	PHENOL	343.20	4.50	19 *
61	67	PHENOL	343.20	9.30	19 *
66	67	PHENOL	343.20	2.30	19 *
72	67	PHENOL	343.20	7.20	19 *
133	67	PHENOL	343.20	39.00	19 *
136	67	PHENOL	343.20	56.50	19 *
102	67	PHENOL	343.20	3.35	19 *
121	67	PHENOL	343.20	12.00	19 *
66	68	ANILINE	343.20	1.79	3 *
65	68	ANILINE	343.20	2.15	15 *
11	68	ANILINE	343.20	1.02	15 *
86	72	CYCLOHEXANE	343.20	9.56	3 *
43	72	CYCLOHEXANE	343.20	12.10	3 *
2	72	CYCLOHEXANE	343.20	1.08	3 *
80	75	METHYL CYCLOPENTANE	343.20	1.17	6 *
91	75	METHYL CYCLOPENTANE	345.00	1.41	68 *
91	75	METHYL CYCLOPENTANE	345.00	1.54	3 *
80	75	METHYL CYCLOPENTANE	345.00	0.99	35 *
66	75	METHYL CYCLOPENTANE	345.00	1.38	3 *
61	75	METHYL CYCLOPENTANE	345.00	1.08	3 *
2	75	METHYL CYCLOPENTANE	345.00	1.07	3 *
35	19	ETHANOL	346.70	2.10	19 *
33	19	ETHANOL	346.70	2.10	19 *
11	48	I-PENTENE	348.00	9.80	3 *
43	36	ETHYL ACETATE	348.20	2.29	3 *
95	41	N-BUTYL BROMIDE	348.20	1.53	3 *
66	47	CYCLOPENTANE	348.20	1.61	26 *
66	61	N-PENTANE	348.20	1.85	26 *
75	66	BENZENE	348.20	1.53	26 *
109	66	BENZENE	348.20	1.62	26 *
61	66	BENZENE	348.20	1.78	26 *
80	66	BENZENE	348.20	1.72	26 *
98	66	BENZENE	348.20	1.69	6 *
94	66	BENZENE	348.20	1.56	26 *
69	66	BENZENE	348.20	1.20	3 *
47	66	BENZENE	348.20	1.40	26 *
66	69	CYCLOHEXENE	348.20	1.17	3 *
91	72	CYCLOHEXANE	348.20	1.55	26 *
66	75	METHYL CYCLOPENTANE	348.20	1.62	26 *
91	75	METHYL CYCLOPENTANE	348.20	1.44	26 *
19	32	2-BUTANONE	349.15	2.08	6 *
12	66	BENZENE	349.30	1.03	3 *
80	2	CARBON TETRACHLORIDE	349.70	1.28	3 *
73	2	CARBON TETRACHLORIDE	349.70	1.11	3 *

SLT	SLV		TEMP	GAMMA INFINITY	REF
85	2	CARBON TETRACHLORIDE	349.70	1.32	3 *
75	2	CARBON TETRACHLORIDE	349.70	1.12	3 *
69	2	CARBON TETRACHLORIDE	349.70	0.95	3 *
66	2	CARBON TETRACHLORIDE	349.70	1.10	3 *
81	2	CARBON TETRACHLORIDE	349.70	1.32	3 *
31	2	CARBON TETRACHLORIDE	349.70	7.40	3 *
82	2	CARBON TETRACHLORIDE	349.70	1.21	3 *
83	2	CARBON TETRACHLORIDE	349.70	1.28	3 *
43	2	CARBON TETRACHLORIDE	349.90	6.50	3 *
21	36	ETHYL ACETATE	350.20	1.18	3 *
31	36	ETHYL ACETATE	350.20	1.90	3 *
19	36	ETHYL ACETATE	350.20	2.22	3 *
37	36	ETHYL ACETATE	350.20	1.07	3 *
72	36	ETHYL ACETATE	350.30	2.29	24 *
68	19	ETHANOL	350.80	2.78	47 *
68	21	ACETONE	350.80	0.96	15 *
68	50	1-PENTENE	350.80	11.20	15 *
50	68	ANILINE	350.80	6.32	15 *
21	68	ANILINE	350.80	0.95	15 *
19	68	ANILINE	350.80	2.21	47 *
6	19	ETHANOL	351.40	1.58	3 *
66	19	ETHANOL	351.40	3.96	3 *
55	19	ETHANOL	351.40	2.33	3 *
72	19	ETHANOL	351.40	7.40	3 *
43	19	ETHANOL	351.40	1.04	3 *
80	19	ETHANOL	351.40	6.80	3 *
21	19	ETHANOL	351.40	1.83	3 *
91	19	ETHANOL	351.40	5.14	3 *
9	19	ETHANOL	351.40	3.55	3 *
126	19	ETHANOL	351.40	14.50	3 *
4	19	ETHANOL	351.40	1.93	3 *
98	19	ETHANOL	351.40	10.90	3 *
37	19	ETHANOL	351.40	2.24	3 *
36	19	ETHANOL	351.40	2.34	3 *
8	19	ETHANOL	351.40	0.99	3 *
56	19	ETHANOL	351.40	2.33	3 *
32	19	ETHANOL	351.40	1.85	3 *
102	19	ETHANOL	351.40	6.25	3 *
62	32	2-BUTANONE	352.80	3.15	3 *
72	32	2-BUTANONE	352.80	3.33	3 *
19	32	2-BUTANONE	352.80	1.79	3 *
2	32	2-BUTANONE	352.80	1.48	3 *
50	32	2-BUTANONE	352.80	2.11	3 *
98	32	2-BUTANONE	352.80	3.15	3 *
4	32	2-BUTANONE	352.80	0.50	3 *
8	32	2-BUTANONE	352.80	2.02	3 *
87	43	N-BUTANOL	353.00	1.08	3 *
47	66	BENZENE	353.10	1.40	3 *

SLT	SLV		TEMP	GAMMA	REF
ID	ID	SOLVENT		INFINITY	
66	1	CARBON DISULFIDE	353.20	1.33	6 *
8	2	CARBON TETRACHLORIDE	353.20	14.10	3 *
36	11	ACETONITRILE	353.20	1.49	12 *
19	31	N-PROPANOL	353.20	1.25	3 *
11	36	ETHYL ACETATE	353.20	1.47	12 *
91	37	DIOXANE	353.20	1.21	3 *
50	37	DIOXANE	353.20	2.12	34 *
98	37	DIOXANE	353.20	3.54	34 *
50	37	DIOXANE	353.20	2.01	3 *
9	37	DIOXANE	353.20	1.26	3 *
109	37	DIOXANE	353.20	3.81	34 *
117	37	DIOXANE	353.20	4.73	3 *
106	37	DIOXANE	353.20	3.03	3 *
98	37	DIOXANE	353.20	3.78	3 *
73	37	DIOXANE	353.20	2.60	3 *
95	37	DIOXANE	353.20	2.25	34 *
80	37	DIOXANE	353.20	3.29	3 *
80	37	DIOXANE	353.20	3.21	34 *
98	44	PYRIDINE	353.20	4.12	3 *
117	44	PYRIDINE	353.20	5.45	3 *
109	44	PYRIDINE	353.20	4.61	3 *
126	44	PYRIDINE	353.20	4.87	3 *
98	55	3-PENTANONE	353.20	2.21	3 *
98	65	CHLOROBENZENE	353.20	1.80	3 *
98	66	BENZENE	353.20	1.66	3 *
108	66	BENZENE	353.20	1.74	3 *
65	66	BENZENE	353.20	0.99	3 *
103	66	BENZENE	353.20	0.95	3 *
94	66	BENZENE	353.20	1.56	3 *
1	66	BENZENE	353.20	1.18	3 *
72	66	BENZENE	353.20	1.45	3 *
133	66	BENZENE	353.20	0.86	3 *
31	66	BENZENE	353.20	5.70	3 *
43	66	BENZENE	353.20	4.46	3 *
68	66	BENZENE	353.20	2.95	3 *
80	66	BENZENE	353.20	1.65	3 *
19	66	BENZENE	353.20	7.37	3 *
87	66	BENZENE	353.20	1.14	3 *
25	66	BENZENE	353.20	2.15	3 *
75	66	BENZENE	353.20	1.43	3 *
94	68	ANILINE	353.20	9.37	3 *
91	68	ANILINE	353.20	2.19	3 *
70	72	CYCLOHEXANE	353.20	2.97	3 *
66	72	CYCLOHEXANE	353.20	1.96	3 *
37	73	1-HEXENE	353.20	2.08	3 *
2	66	BENZENE	353.30	1.11	3 *
4	66	BENZENE	353.30	0.85	3 *
32	66	BENZENE	353.30	1.27	3 *

SLT	SLV		TEMP	GAMMA INFINITY	REF
	ID	SOLVENT			
8	66	BENZENE	353.30	8.95	3 *
18	66	BENZENE	353.30	0.83	3 *
37	66	BENZENE	353.30	1.10	3 *
21	66	BENZENE	353.30	1.65	3 *
44	66	BENZENE	353.30	1.29	3 *
14	66	BENZENE	353.30	1.02	3 *
79	43	N-BUTANOL	353.40	2.09	3 *
19	72	CYCLOHEXANE	353.90	13.60	3 *
66	72	CYCLOHEXANE	353.90	1.42	3 *
65	72	CYCLOHEXANE	353.90	1.70	3 *
21	72	CYCLOHEXANE	353.90	5.02	3 *
61	72	CYCLOHEXANE	353.90	1.19	3 *
44	72	CYCLOHEXANE	353.90	2.81	3 *
91	72	CYCLOHEXANE	353.90	1.40	3 *
43	72	CYCLOHEXANE	353.90	11.52	3 *
98	72	CYCLOHEXANE	353.90	1.03	3 *
80	72	CYCLOHEXANE	353.90	1.06	3 *
31	72	CYCLOHEXANE	353.90	10.03	3 *
21	72	CYCLOHEXANE	353.90	4.10	3 *
14	72	CYCLOHEXANE	353.90	2.62	3 *
8	72	CYCLOHEXANE	353.90	8.90	3 *
36	72	CYCLOHEXANE	353.90	2.57	24 *
43	14	1,2-DICHLOROETHANE	354.20	3.23	3 *
31	14	1,2-DICHLOROETHANE	354.20	3.73	3 *
66	11	ACETONITRILE	354.80	2.49	3 *
62	11	ACETONITRILE	354.80	10.70	3 *
46	11	ACETONITRILE	354.80	3.35	3 *
91	11	ACETONITRILE	354.80	3.05	3 *
103	11	ACETONITRILE	354.80	4.05	3 *
102	11	ACETONITRILE	354.80	4.25	3 *
14	69	CYCLOHEXENE	355.10	1.96	3 *
2	69	CYCLOHEXENE	355.10	0.93	3 *
66	14	1,2-DICHLOROETHANE	356.60	1.04	3 *
91	14	1,2-DICHLOROETHANE	356.60	1.09	3 *
21	14	1,2-DICHLOROETHANE	356.60	0.81	3 *
69	14	1,2-DICHLOROETHANE	356.60	1.86	3 *
72	14	1,2-DICHLOROETHANE	356.60	2.99	3 *
72	19	ETHANOL	363.15	6.40	19 *
66	32	2-BUTANONE	363.15	1.05	19 *
108	64	NITROBENZENE	363.15	5.95	39 *
133	19	ETHANOL	363.20	27.50	19 *
126	19	ETHANOL	363.20	15.00	19 *
107	19	ETHANOL	363.20	9.50	19 *
136	19	ETHANOL	363.20	40.00	19 *
123	19	ETHANOL	363.20	13.20	19 *
42	19	ETHANOL	363.20	6.60	19 *
102	19	ETHANOL	363.20	7.40	19 *
98	21	ACETONE	363.20	3.60	19 *

SLT	SLV	SOLVENT	TEMP	GAMMA INFINITY	REF
126	31	N-PROPANOL	363.20	8.74	3 *
107	32	2-BUTANONE	363.20	3.00	19 *
123	32	2-BUTANONE	363.20	3.40	19 *
126	32	2-BUTANONE	363.20	3.10	19 *
44	43	N-BUTANOL	363.20	0.76	3 *
43	44	PYRIDINE	363.20	0.95	3 *
98	56	2-PENTANONE	363.20	2.84	3 *
123	67	PHENOL	363.20	10.00	19 *
126	67	PHENOL	363.20	16.50	19 *
91	67	PHENOL	363.20	2.55	19 *
102	67	PHENOL	363.20	3.10	19 *
72	67	PHENOL	363.20	6.20	19 *
66	67	PHENOL	363.20	2.07	19 *
120	67	PHENOL	363.20	3.50	19 *
107	67	PHENOL	363.20	8.30	19 *
133	67	PHENOL	363.20	32.00	19 *
136	67	PHENOL	363.20	44.50	19 *
98	67	PHENOL	363.20	10.00	19 *
61	67	PHENOL	363.20	7.80	19 *
94	68	ANILINE	363.20	8.38	3 *
91	68	ANILINE	363.20	2.15	3 *
61	11	ACETONITRILE	363.30	9.00	3 *
59	31	N-PROPANOL	367.60	2.00	19 *
14	31	N-PROPANOL	368.10	2.93	3 *
57	31	N-PROPANOL	368.20	1.80	19 *
98	55	3-PENTANONE	368.20	2.08	3 *
58	31	N-PROPANOL	368.40	1.80	19 *
117	44	PYRIDINE	369.80	4.82	3 *
102	31	N-PROPANOL	370.30	3.76	3 *
72	31	N-PROPANOL	370.30	3.80	3 *
43	31	N-PROPANOL	370.30	1.06	3 *
57	31	N-PROPANOL	370.30	1.76	3 *
2	31	N-PROPANOL	370.30	3.30	3 *
66	31	N-PROPANOL	370.30	3.30	3 *
65	31	N-PROPANOL	370.30	3.45	3 *
80	31	N-PROPANOL	370.30	6.47	3 *
35	31	N-PROPANOL	370.30	2.41	3 *
94	31	N-PROPANOL	370.30	4.62	3 *
37	31	N-PROPANOL	370.30	1.80	3 *
36	31	N-PROPANOL	370.30	1.69	3 *
98	31	N-PROPANOL	370.30	7.20	3 *
91	31	N-PROPANOL	370.30	3.51	3 *
31	57	N-PROPYL ACETATE	370.30	1.83	3 *
66	31	N-PROPANOL	370.40	2.50	55 *
32	8	METHANOL	373.15	1.96	19 *
21	8	METHANOL	373.15	1.66	19 *
36	19	ETHANOL	373.15	2.00	19 *
80	19	ETHANOL	373.15	8.40	19 *

SLT	SLV		TEMP	GAMMA INFINITY	REF
	ID	SOLVENT			
98	32	2-BUTANONE	373.15	2.88	19 *
32	43	N-BUTANOL	373.15	1.42	19 *
97	8	METHANOL	373.20	3.59	19 *
55	8	METHANOL	373.20	2.45	19 *
115	8	METHANOL	373.20	5.20	19 *
91	43	N-BUTANOL	373.20	2.56	3 *
97	43	N-BUTANOL	373.20	1.72	3 *
126	43	N-BUTANOL	373.20	8.86	3 *
79	43	N-BUTANOL	373.20	1.80	3 *
68	63	1-PENTANOL	373.20	1.72	3 *
102	64	NITROBENZENE	373.20	1.61	3 *
91	64	NITROBENZENE	373.20	1.46	3 *
120	64	NITROBENZENE	373.20	1.87	3 *
98	65	CHLOROBENZENE	373.20	1.73	3 *
94	68	ANILINE	373.20	6.68	3 *
91	68	ANILINE	373.20	2.06	3 *
63	68	ANILINE	373.20	2.40	3 *
102	68	ANILINE	373.20	2.32	3 *
8	56	2-PENTANONE	373.30	2.95	3 *
19	56	2-PENTANONE	373.30	2.30	3 *
19	55	3-PENTANONE	374.10	2.33	3 *
8	55	3-PENTANONE	374.10	2.08	3 *
19	9	NITROMETHANE	374.40	3.55	3 *
51	9	NITROMETHANE	374.40	8.00	3 *
19	37	DIOXANE	374.50	1.97	3 *
43	37	DIOXANE	374.50	1.51	3 *
66	37	DIOXANE	374.50	1.14	3 *
36	37	DIOXANE	374.50	1.08	3 *
31	37	DIOXANE	374.50	1.73	3 *
73	37	DIOXANE	374.50	2.52	33 *
67	78	CYCLOHEXANOL	375.60	0.29	3 *
70	67	PHENOL	381.00	0.11	3 *
72	19	ETHANOL	383.15	6.00	19 *
91	63	1-PENTANOL	383.20	2.60	3 *
65	78	CYCLOHEXANOL	383.20	1.69	3 *
126	44	PYRIDINE	384.70	3.83	3 *
78	67	PHENOL	385.00	0.30	3 *
68	8	METHANOL	385.20	2.61	15 *
8	68	ANILINE	385.20	1.98	15 *
68	19	ETHANOL	385.70	2.41	47 *
68	21	ACETONE	386.70	1.21	15 *
21	68	ANILINE	386.70	1.25	15 *
19	68	ANILINE	386.70	1.92	47 *
98	16	NITROETHANE	387.20	6.19	3 *
91	44	PYRIDINE	388.40	1.26	3 *
8	44	PYRIDINE	388.40	1.05	3 *
66	44	PYRIDINE	388.40	1.18	3 *
14	43	N-BUTANOL	388.80	2.27	3 *

SLT	SLV		TEMP	GAMMA INFINITY	REF
	ID	SOLVENT			
36	43	N-BUTANOL	389.00	1.79	3 *
78	43	N-BUTANOL	390.20	1.10	3 *
72	43	N-BUTANOL	390.20	3.27	3 *
65	43	N-BUTANOL	390.20	2.45	3 *
102	43	N-BUTANOL	390.20	2.68	3 *
37	43	N-BUTANOL	390.20	1.14	3 *
80	43	N-BUTANOL	390.20	2.84	3 *
66	43	N-BUTANOL	390.20	2.28	3 *
103	43	N-BUTANOL	390.20	2.73	3 *
34	43	N-BUTANOL	390.20	1.22	3 *
19	43	N-BUTANOL	390.80	1.00	3 *
4	43	N-BUTANOL	390.80	1.46	3 *
8	43	N-BUTANOL	390.80	1.33	3 *
31	43	N-BUTANOL	390.80	0.99	3 *
21	43	N-BUTANOL	390.80	1.93	3 *
98	43	N-BUTANOL	390.90	3.99	56 *
2	43	N-BUTANOL	391.00	2.60	3 *
91	11	ACETONITRILE	393.20	3.02	12 *
68	11	ACETONITRILE	393.20	1.35	15 *
19	11	ACETONITRILE	393.20	2.20	12 *
36	11	ACETONITRILE	393.20	1.42	12 *
11	19	ETHANOL	393.20	2.05	12 *
11	36	ETHYL ACETATE	393.20	1.42	12 *
11	68	ANILINE	393.20	1.05	15 *
101	67	PHENOL	393.30	0.31	3 *
103	65	CHLOROBENZENE	402.00	0.89	3 *
72	19	ETHANOL	403.15	5.60	19 *
72	32	2-BUTANONE	403.20	2.25	19 *
121	32	2-BUTANONE	403.20	3.65	19 *
121	67	PHENOL	403.20	1.40	19 *
72	67	PHENOL	403.20	4.80	19 *
66	67	PHENOL	403.20	1.75	19 *
65	78	CYCLOHEXANOL	403.20	1.60	3 *
66	65	CHLOROBENZENE	404.80	1.11	3 *
31	65	CHLOROBENZENE	404.80	2.98	3 *
43	65	CHLOROBENZENE	404.80	2.53	3 *
80	65	CHLOROBENZENE	404.80	1.59	3 *
72	65	CHLOROBENZENE	404.80	1.33	3 *
8	65	CHLOROBENZENE	404.80	4.94	3 *
19	65	CHLOROBENZENE	404.80	4.19	3 *
21	65	CHLOROBENZENE	404.90	1.39	20 *
103	63	1-PENTANOL	411.00	2.04	3 *
8	63	1-PENTANOL	411.00	1.33	3 *
101	67	PHENOL	424.30	0.36	3 *
104	25	DIMETHYL FORMAMIDE	426.20	2.57	3 *
103	25	DIMETHYL FORMAMIDE	426.20	2.82	3 *
8	25	DIMETHYL FORMAMIDE	426.20	0.63	3 *
61	25	DIMETHYL FORMAMIDE	426.50	5.80	3 *

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SLT	SLV		TEMP	GAMMA	REF	
ID	ID	SOLVENT		INFINITY		
32	67	PHENOL	429.00	0.33	3	*
43	78	CYCLOHEXANOL	432.00	0.93	3	*
70	78	CYCLOHEXANOL	433.80	1.12	3	*
68	78	CYCLOHEXANOL	434.20	1.33	3	*
128	67	PHENOL	455.00	7.42	3	*
79	67	PHENOL	455.00	0.46	3	*
109	67	PHENOL	455.00	9.76	3	*
91	67	PHENOL	455.00	2.07	3	*

* These data are extrapolated

ERT Database Evaluation

Kevin Stephenson
15 April 1988

An error analysis has been completed on the MOSCED equation γ^m predictions (1) as measured against three separate experimental data sets of γ^m values. Each successive data set was a subset of the previous data set with some of the less reliable values removed. This analysis was performed for the purpose of determining which of the data sets was most suitable for reparameterizing the acidity/basicity term of the MOSCED equation, i.e. from which data set did MOSCED show the least error (see Figure 1). All of the data sets were compiled on Lotus 123 spreadsheets and the MOSCED equation was evaluated with formulas in these worksheets.

The first data set examined was one very similar to that used by Gene Thomas in developing the MOSCED equation. The database contained 3341 records as opposed to the 3387 used by Thomas(1). The discrepancy lies in the fact that some inconsistencies in the Thomas database, which were presumed to be typographical errors, were not included. MOSCED showed an average error of 11.70% when compared with this database, which differs from the 9.1% error reported by Thomas. At the present, the source of this difference has not been identified. Hand calculations to double check the calculations of MOSCED have not revealed any mistakes, and the MOSCED parameters appear to be the same as those used by Thomas. In any case, the discrepancy is not critical since the focus of this study is on the relative errors produced when MOSCED is compared to each data set.

The second data set under consideration was composed of the first data set minus those records which represented extrapolated values. By removing the extrapolated values it was expected that the accuracy of MOSCED relative to the measured values would increase. This database consisted of 1997 records and resulted in an average error of 9.53%, a large improvement over the initial database.

The final database considered consisted of those records in the second data set which had been measured at 293-298°K. As before, removing these data reduced the approximations made by MOSCED and was expected to provide greater accuracy. As expected, this database of 881 records resulted in an average error of 9.14% - comparable to the second data set and again better than the initial data set.

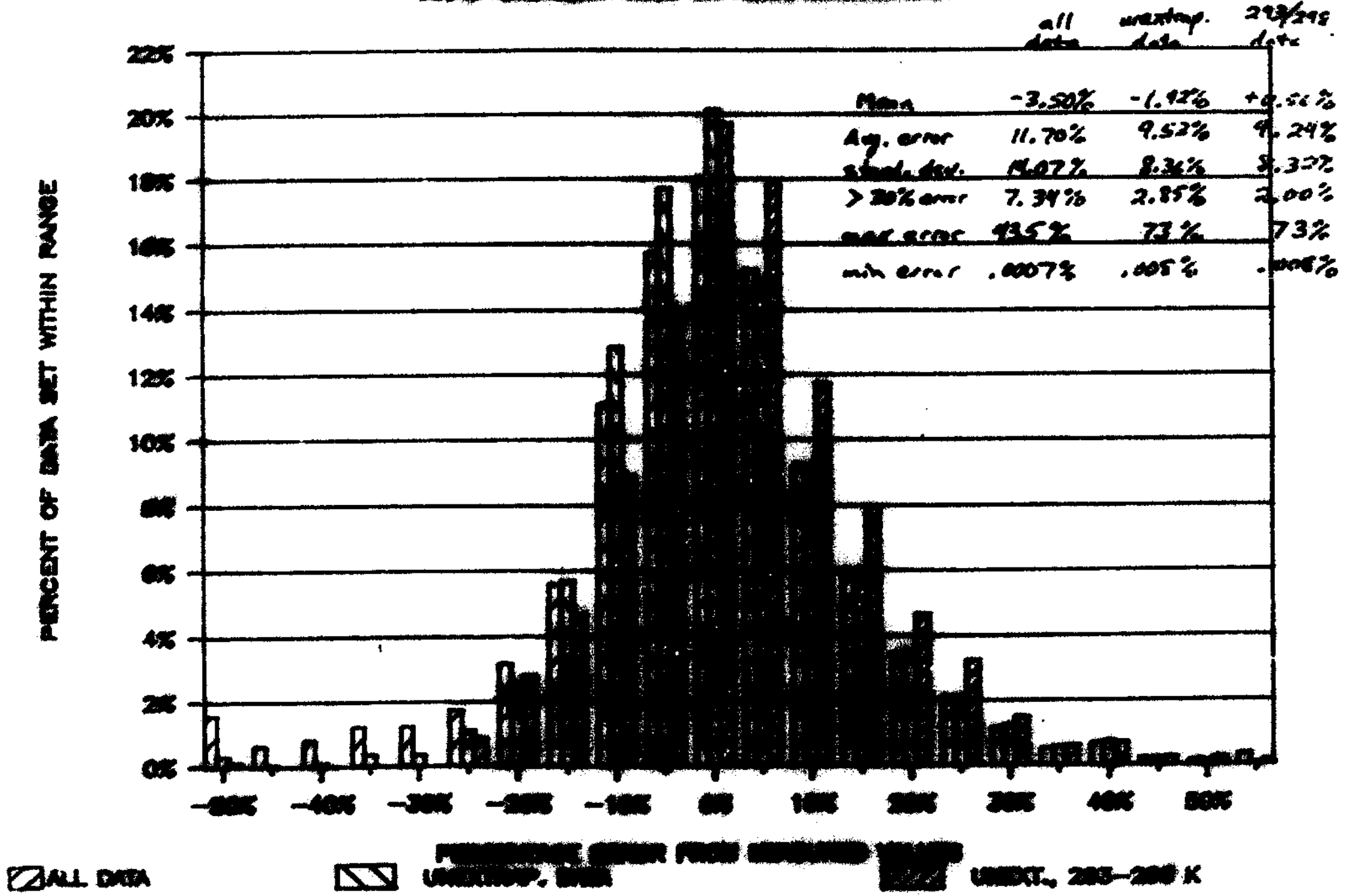
From these results it was concluded that the first data set should not be used in the reparameterization since the large degree of uncertainty in the extrapolated values resulted in a significantly higher error on the part of MOSCED. It should be noted here that even this 11.70% error is almost as good as can be expected since the measured data is only accurate to approximately $\pm 10\%$. The latter two data sets are quite similar in the errors produced. It is difficult to differentiate between them based only on this criteria, especially since the average errors produced are very close to the limits imposed by the data.

Due to this, both will be utilized in the reparameterization process.

The attached figure (Figure 1) is a histogram of the relative error of NOCED when compared with each of the data sets discussed. It can be seen that each analysis produced a nearly normal distribution. It should also be noted that the first (largest) data set not only gave a larger average error but also resulted in many more errors of greater than 30%. This can be attributed to the uncertainty inherent in the extrapolated data of this data set.

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Figure 1
PERCENT OF DATA SET WITHIN RANGE



References

1. Thomas, E. R., and G. A. Eckert. Prediction of limiting activity coefficients by a modified separation of Coulomb energy. Journal of Chemical Physics, 1954, 22, 194.


```
program msdftvx
c
c *****
c
c   this program is used to fit mosced equation parameters in
c   fmsl routine zxmwd on the school of chemical science
c
c   this program modifies the acidity/basicity term in mos
c   incorporating the kamlet-taft alpha/beta data base
c
c   with the modification of the acidity/basicity term, the
c   coefficients of all the other terms in mosced must be
c   refit. therefore, this program is a multiparameter fit
c
c
c   developed by: wayne j. howell
c   modified by: kevin m. stephenson
c
c   version: 2.00
c   date: 20 Apr 1988
c
c *****
c
c *****
c declare external subroutine used in fmsl
c *****
c
c   external msdffit
c
c *****
c declare variables used in fmsl
c *****
c
c   double precision g,t,data,ri,v,q,akt,bkt,x(20),gamc1c,
c   1          lamda1,lamda2,tau1,tau2,a1,a2,
c   2          b1,b2,d12,ps11,x11
c
c   double precision work(1500),lower,upper
c
c *****
c define variables
c *****
c
c   integer npar,ndata,nsrch,n1,iwork(20),ier
c
c   common ndata
c   common gamc1c(500)
c
c   common /count/npar
```

```
c
c *****
c call imsl: zxmwd to determine x(1), x(2), x(3)
c *****
c
c   write(*,*) 'npar =',npar
c   write(*,*) 'ndata =',ndata
c   write(*,*) 'nsrch =',nsrch
c   write(*,*)
c
c   call zxmwd(mscdfit,npar,nsig,lower,upper,nsrch,
c 1          x,g,work,iwork,ier)
c
c   write(*,*)' ***** finished imsl *****'
c
c *****
c set parameters from imsl: zxmwd for output
c *****
c
c   ierm = ier
c
c *****
c call output subroutine
c *****
c
c   call output(solute,solvent,name)
c
c *****
c end of main program
c *****
c
c   stop
c   end
c
c
c
c *****
c *****
c subroutine section
c *****
c *****
c
c
c
c
```

```
c
c*****
c input subroutine: rdat
c*****
c
c   subroutine rdat(solute,solvent,name)
c
c   double precision t,data,ri,v,q,akt,bkt,x(20),gamma(i),
1      lower,upper
c
c   integer npar,ndata
c
c   common ndata
c   common gamma:c(500)
c
c   common/count/npar
c   common/ident/iv(500),iv(500),id(500)
c   common/gamma/t(500),data(500)
c   common/prop/ri(500),v(500),q(500)
c   common/kt/akt(500),bkt(500)
c   common/cnums/igrp(500),igtg(500),inum(500)
c   common/ins11/x,nsrch
c   common/ins12/lower(20),upper(20)
c
c   character * 27 solute(500),solvent(500),name(500)
c
c***** read in initial values for parameters: x(i) *****
c
c   do 1000 i = 1,20
c
c
c
c
c   read(8,15)lower(i)
c   write(11,15)lower(i)
c   read(9,15)upper(i)
c   write(12,15)upper(i)
c   if(lower(i).eq.999.or.upper(i).eq.999)go to 55
c   write(*,*) lower(i),upper(i)
c
c
c   npar = i
c
c   15   format(f9.5)
```

```
C
C 1000 continue
C
C ***** read in gamma data from gamma.dat *****
C
C 55 continue
C
C write(*,*)
C
C do 100 ia = 1,500
C   read(2,10) iu(ia),solute(ia),iv(ia),solvent(ia),t(ia),data(ia)
C   write(6,10) iu(ia),solute(ia),iv(ia),solvent(ia),t(ia),data(ia)
C
C   if(iu(ia) .eq. 999 .and. iv(ia) .eq. 999) go to 50
C
C   ndata = ia
C
C 100 continue
C
C 10 format(13,1x,a23,1x,13,1x,a25,1x,f6.2,3x,f6.2)
C
C 50 continue
C
C ***** read in physical properties and other data from propty.dat *****
C
C
C do 110 l = 1,144
C   read(1,20) r1(l),v(l),q(l),akt(l),bkt(l),igrp(l),igtp(l),
C   l          inum(l),id(l),name(l)
C
C   write(5,20) r1(l),v(l),q(l),akt(l),bkt(l),igrp(l),igtp(l),
C   l          inum(l),id(l),name(l)
C
C 110 continue
C
C 20 format(f5.3,1x,f5.1,1x,f5.2,1x,f5.2,1x,f5.2,2x,f2.2x,13,
C   l       2x,13,1x,13,1x,a25)
C
C
C RETURN
C END
C
C *****
C fmsl: zxsq external subroutine: msdfit
C *****
C
```

```
subroutine mscdfit(npar,x,g)
c
c double precision g,lngam2,t,data,r1,v,q,akt,bkt,gamc ic,
1      lamda1,lamda2,tau1,tau2,a1,a2,b1,lower,
2      b2,d12,ps11,xi1,x(20),r11,r12,v1,v2,q1,q2,
3      akt1,akt2,bkt1,bkt2,erat,taut,tau2t,a1t,a2t,
4      b1t,b2t,aa,pol,term1,term2,term3,sum,errsq,
5      upper
c
c integer npar,ndata
c
c common ndata
c common gamc ic(500)
c
c common/ident/1u(500),1v(500),1d(500)
c common/gamma/t(500),data(500)
c common/prop/r1(500),v(500),q(500)
c common/kt/akt(500),bkt(500)
c common/cnms/igrp(500),igtp(500),inum(500)
c common/mscd/lamda1(500),lamda2(500),tau1(500),tau2(500),
1      a1(500),a2(500),b1(500),b2(500),
2      d12(500),ps11(500),xi1(500)
c common/ims12/lower(20),upper(20)
c
c character * 27 solute(500),solvent(500),name(500)
c g = 0.0
c
c
c ***** begin ims1 loop *****
c
c write(*,*) x(1),x(2)
c
c do 100 ic = 1, ndata
c
c     ***** set properties *****
c
c     1su = 1u(ic)
c     1sv = 1v(ic)
c
c     r12 = r1(1su)
c     r11 = r1(1sv)
c
c     v2 = v(1su)
c     v1 = v(1sv)
c
c     q2 = q(1su)
c     q1 = q(1sv)
```

```
c
      akt2 = akt(isu)
      akt1 = akt(isv)
c
      bkt2 = bkt(isu)
      bkt1 = bkt(isv)
c
      ***** determine parameters at 293K *****
c
      lambda2(ic) = x(1)*((r12**2 - 1.)/(r12**2 + 2.))
      lambda1(ic) = x(1)*((r11**2 - 1.)/(r11**2 + 2.))
c
      tau2(ic) = x(3)*(4.5/(3.5 + inum(isu)))*(1. + inum(isu)/100.)
      tau1(ic) = x(3)*(4.5/(3.5 + inum(isv)))*(1. + inum(isv)/100.)
c
      a2(ic) = x(4)*akt2/v2
      a1(ic) = x(4)*akt1/v2
c
      b2(ic) = x(5)*bkt2/v2
      b1(ic) = x(5)*bkt1/v2
c
      ***** determine parameters at temperature of exptl data *****
c
      trat = 293.0/t(ic)
c
      tau2t = tau2(ic)*trat**0.4
      tau1t = tau1(ic)*trat**0.4
c
      a2t = a2(ic)*trat**0.8
      a1t = a1(ic)*trat**0.8
c
      b2t = b2(ic)*trat**0.8
      b1t = b1(ic)*trat**0.8
c
      ***** determine combinatorial term *****
c
      aa = x(2)
      aa = x(6) - x(7)*(tau2t**2 + a2t*b2t)
c
      d12(ic) = aa*dlog(v2/v1) + 1. - (v2/v1)**aa
c
      ***** determine asymmetry terms *****
c
      pol = q1**4*(x(8) - x(9)*dexp(-1.*x(10)*tau1t**3)) + 1.
c
      ps11(ic) = pol + x(11)*a1t*b1t
c
```

```
C      x11(ic) = x(12)*(po1 - 1.) +
C      1          (x(13) - x(14)*dexp((a1(ic)*b1(ic))**1.5*
C      2          (-1.*x(15))))**(trat**2)
C
C      ***** calculate gamma-inf using mosced equation *****
C
C      term1 = (lamda1(ic) - lamda2(ic))**2
C
C      term2 = (q1*q2*(taut1 - tau2t))**2/ps11(ic)
C
C      term3 = (a1t - a2t)*(b1t - b2t)/x11(ic)
C
C      sum = term1 + term2 + term3
C
C      lngam2 = v2*term1/(1.987*t(ic)) + d12(ic)
C      lngam2 = v2*sum/(1.987*t(ic)) + d12(ic)
C
C      ***** define objective function *****
C
C      gamc1c(ic) = dexp(lngam2)
C      errsq = (gmc1c(ic) - data(ic))**2
C
C      g = g + errsq
C
C      ***** end imsl loop *****
C
C      100 continue
C
C      ***** end of subroutine moscdfit *****
C
C      RETURN
C      END
C
C
C      *****
C      subroutine output
C      *****
C
C      subroutine output(solute,solvent,name)
C
C      double precision t,data,r1,v,q,akt,bkt,x(20),lamda1,lamda2,
C      1          tau1,tau2,a1,a2,b1,b2,d12,ps11,x11,
C      2          gamc1c,error(500),toterr,avgerr,maxerr,minerr,
C      3          lower,upper
```

```
c integer ndata
c
c common ndata
c common gamc1c(500)
c
c common/ident/iv(500),iv(500),id(500)
c common/gamma/t(500),data(500)
c common/prop/ri(500),v(500),q(500)
c common/kt/akt(500),bkt(500)
c common/cnums/igrp(500),igtp(500),inum(500)
c common/ims11/x,nrch
c common/ims12/lower(20),upper(20)
c common/mscd/lambda1(500),lambda2(500),tau1(500),tau2(500),
1      a1(500),a2(500),b1(500),b2(500),
2      d12(500),ps11(500),x11(500)
c
c character * 27 solute(500),solvent(500),name(500)
c
c *****
c calculate percent error
c *****
c
c maxerr = 0
c minerr = 0
c toterr = 0
c
c do 1000 i = 1,ndata
c   error(i) = ((dabs(data(i) - gamc1c(i)))/data(i))*100
c   toterr = toterr + error(i)
c   if (error(i).gt.maxerr) maxerr = error(i)
c   if (i.eq.1) minerr = error(i)
c   if (error(i).lt.minerr) minerr = error(i)
c
c 1000 continue
c
c avgerr = toterr/ndata
c
c *****
c print results
c *****
c ***** create solute and solvent identification table *****
c
c do 2000 i = 1,ndata
c   write(3,10) iv(i),solute(i),iv(i),solvent(i)
```



```
10      Format(13,1x,a27,1x,i3,1x,a27)
2000 continue
c
c*****check MOSCED parameters used by IMSL*****
c
c
c      do 3000 i=1,144
c          write(10,15) r(i),v(1),q(1),akt(1),bkt(1),igrp(1),
c              1          igtb(i),inum(1),id(1),name(1)
c
c      15      format(f5.3,1x,f5.1,1x,f5.2,1x,f5.2,1x,f5.2,2x,i2,2x,i3,
c              1          2x,i3,1x,i3,1x,a25)
c
c      3000    continue
c
c      ##### imsl convergence criteria #####
c
c      write(4,30)
c      30      format(' ***** imsl convergence ***** ',/)
c
c      write(4,40)form
c      40      format('                IMSL IER :',i3)
c
c      ***** write mosced parameters values fit with imsl *****
c
c      write(4,80)
c      80      format(' ***** parameter values ***** ',/)
c
c      write(4,90)x(1),lower(1),upper(1)
c      90      format('x(1) :',g15.5,' lower(1) :',g15.5,' upper(1) :',g15.5)
c      write(4,110)x(2)
c      110     format('                x(2) :',g15.5)
c      write(4,120)x(3)
c      120     format('                x(3) :',g15.5)
c      write(4,130)x(4)
c      130     format('                x(4) :',g15.5)
c      write(4,140)x(5)
c      140     format('                x(5) :',g15.5)
c      write(4,150)x(6)
c      150     format('                x(6) :',g15.5)
c      write(4,160)x(7)
c      160     format('                x(7) :',g15.5)
c      write(4,170)x(8)
c      170     format('                x(8) :',g15.5)
c      write(4,180)x(9)
c      180     format('                x(9) :',g15.5)
c      write(4,190)x(10)
```

```
190 format(' x(10) :',g15.5)
write(4,200)x(11)
200 format(' x(11) :',g15.5)
write(4,210)x(12)
210 format(' x(12) :',g15.5)
write(4,220)x(13)
220 format(' x(13) :',g15.5)
write(4,230)x(14)
230 format(' x(14) :',g15.5)
write(4,240)x(15)
240 format(' x(15) :',g15.5,///)
c
write(4,600)
write(4,700) average, maxerr, minerr
600 format(' AVERAGE ERROR MAX ERROR MIN ERROR')
700 format(10x,f7.3,8x,f7.3,9x,f7.3,///)
c
c***** write gamma data and percent error *****
c
do 300 i = 1,ndata
write(4,20) iu(i), iv(i), data(i), gamma(i), error(i)
20 format(13,2x,13.5x,f6.2,5x,f6.2,5x,f6.2,5x)
300 continue
c
c***** write mosed parameter values *****
c
do 400 i = 1,ndata
write(7,500)iu(i), solute(i), t(i), lambda2(i), tau2(i), a2(i),
1 akt(iu(i)), b2(i), bkt(iu(i))
write(7,500)iv(i), solvent(i), t(i), lambda1(i), tau1(i), a1(i),
1 akt(iv(i)), b1(i), bkt(iv(i))
c
500 format(13,2x,a27,2x,f6.2,2x,f5.3,2x,f6.3,2x,f5.3,2x,f5.3,
1 2x,f5.3,2x,f5.3)
c
400 continue
c
c***** end of subroutine output *****
c
return
end
```

Mar 1987

The IMSL Library

SCS.RF-2.17.1

IMSL (International Mathematical & Statistical Libraries) is an extensive collection of mathematical and statistical subroutines written in FORTRAN. It is organized into the following sections:

- Analysis of Variance
- Basic Statistics
- Categorized Data Analysis
- Differential Equations; Quadrature; Differentiation
- Eigenystem Analysis
- Forecasting; Econometrics; Time Series; Transforms
- Generation and Testing of Random Numbers
- Interpolation; Approximation; Smoothing
- Linear Algebraic Equations
- Mathematical and Statistical Special Functions
- Non-Parametric Statistics
- Observation Structure; Multivariate Statistics
- Regression Analysis
- Sampling
- Utility Functions
- Vector-Matrix Arithmetic
- Trees and Networks; Linear Programming

The VAX currently has Edition 9.2 of the IMSL Library in both single and double precision versions. The documentation consists of a 4 volume manual available in room 103 Hayes (The documentation is the Edition 9). To find a routine to fill a particular need, it is best to examine the SYNOC INDEX in the first volume of the manual. Each IMSL routine is identified by several keywords. The keywords are arranged alphabetically with the name of the routine in the right-hand column. For example, if you wanted a routine to do a least-squares approximation by cubic splines you could look up any of the keywords least squares, approximation or spline. If you just want to see what least-squares routines are available, look under least squares. The documentation on each routine is arranged alphabetically by routine name.

To use IMSL in your program you must LINK the library with your program. Add ,IMSL/LIB or ,IMSL/LIB to the list of object modules being linked if you want the single precision library. Add ,IMSLD/LIB to link in the double precision library.

Format:

```
0 LINK my-prog,IMSL/LIB
```

Example:

```
0 LINK SOLVEIT,IMSL/LIB
0 LINK ORGVAL,FITCURVE,IMSLD/LIB
```

IMSL, IMSL and IMSLD are system-wide logical names which will always point to the appropriate libraries.

The complete source code for the single and double precision libraries is usually available on line in the directory \$SOURCE\$(IMSL). However, it may be deleted if disk space is tight. It will always be available on magnetic tape.

IMSL ROUTINE NAME - EXMND

PURPOSE - GLOBAL MINIMUM (WITH CONSTRAINTS) OF A FUNCTION OF N VARIABLES

USAGE - CALL EXMND(FCN,N,NSIG,A,B,NSRCH,X,F,WORK, IWORK, IER)

ARGUMENTS

FCN - A USER SUPPLIED SUBROUTINE WHICH CALCULATES F GIVEN X(1),X(2),...,X(N). FCN IS REFERENCED AS FOLLOWS,
CALL FCN(N,X,F)
WHERE X IS A VECTOR OF LENGTH N
FCN MUST APPEAR IN AN EXTERNAL STATEMENT IN THE CALLING PROGRAM.
FCN MUST NOT ALTER THE VALUES OF X(1),...,X(N), OR N.

N - THE NUMBER OF INDEPENDENT PARAMETERS. (INPUT)

NSIG - CONVERGENCE SIGNIFICANCE. (INPUT) NSIG IS THE NUMBER OF SIG FIGS OF ACCURACY REQUIRED IN THE PARAMETER ESTIMATES.

A,B - CONSTRAINT VALUES OF LENGTH N. (INPUT) X(I) IS REQUIRED TO SATISFY -
 $A(I) \leq X(I) \leq B(I)$

NSRCH - NUMBER OF SEARCH STEPS TO BE GENERATED. (INPUT) SUGGESTED VALUE = MIN(2*N+5,100)

X - VECTOR OF LENGTH N CONTAINING THE FINAL PARAMETER ESTIMATES. (OUTPUT)

F - VALUE OF THE FUNCTION AT THE FINAL PARAMETER ESTIMATES. (OUTPUT)

WORK - REAL WORK VECTOR OF LENGTH N*(2+1)/3+11*N. AN OUTPUT OF THE NUMBER OF SIGNIFICANT DIGITS IN THE FINAL PARAMETER ESTIMATES IS RETURNED IN WORK(1).

IWORK - INTEGER WORK VECTOR OF LENGTH N

IER - ERROR PARAMETER (OUTPUT)

TRUNCAL ERROR

IER = 1: INDICATES THAT THE ALGORITHM HAS CONVERGED TO A POINT WHICH MAY ONLY BE A SINGLE POINT.

IER = 2: INDICATES THAT IT WAS NOT POSSIBLE TO ENFORCE THE CONSTRAINTS TO HIGH ENOUGH ACCURACY.

IER = 3: INDICATES THAT THE ITERATION WAS UNSTABLE AFTER 100*(N+1) FUNCTION EVALUATIONS AND STOPPED.

IER = 4: INDICATES THAT X(1),...,X(N) FOR SOME I=1,...,N. NO ATTEMPT IS MADE TO FIND THE MINIMUM IN THIS CASE.

PRECISION/MESSAGE - SINGLE AND DOUBLE PRECISION
- SINGLE/115, 244, 100

REQD. INCL ROUTINES - UMINF, UMINF, UMINF, UMINF, UMINF, UMINF

NOTATION - INFORMATION ON SPECIAL NOTATION AND CONVENTIONS IS AVAILABLE IN THE MANUAL
IDENTIFICATION OF OTHER IMSL ROUTINE CALLS

REMARKS

WHEN IER IS RETURNED AS 130 OR 131, THE PARAMETER ESTIMATES IN X MAY NOT BE RELIABLE. FURTHER CHECKING SHOULD BE PERFORMED. USE OF A LARGER NSRCH VALUE MAY PRODUCE MORE RELIABLE PARAMETER ESTIMATES.

Algorithm

The constrained minimization problem is equivalent to

$$\text{minimize } f(a_1+(b_1-a_1)\sin^2 t_1, \dots, a_n+(b_n-a_n)\sin^2 t_n) \\ (t_1, \dots, t_n)$$

where the t_i are now unconstrained. With this transformation, in fact, each possible global minimum, including any on the boundary, is transformed into a local minimum.

MINSD calls a modified version of MINN to do about 4 iterations with each of NSRCH starting points (generated by ISRCH). The five which result in the lowest values of the function are allowed to continue to convergence. The local minimum found which, of these five, gives the lowest function value is taken to be the global minimum. As NSRCH is increased, the probability that this point is really the global minimum is increased.

See references:

1. Box, M. J., "A comparison of several current optimization methods, and the use of transformations in constrained problems", Computer Journal (9) 1966, 67-77.

Example

The minimum of $f(x_1, x_2, x_3, x_4, x_5) = x_1^2 + x_2^2 + x_3^2 + x_4^2 + x_5^2$ is desired in the hyper-rectangle

$$\begin{aligned} -1 \leq x_1 \leq 0 \\ -1 \leq x_2 \leq 2 \\ -2 \leq x_3 \leq 1 \\ 0 \leq x_4 \leq 3 \\ 2 \leq x_5 \leq 3 \end{aligned}$$

Input:

```
REAL A(5), B(5), X(5), WORK(70), F
INTEGER N, NSIG, NSRCH, INCRN(5), IER
EXTERNAL FCN
N = 5
NSIG = 1
NSRCH = 10
A = [-1.0, -1.0, -2.0, 0.0, 2.0]
B = [0.0, 2.0, 1.0, 3.0, 3.0]
CALL MINSD (FCN, N, NSIG, A, B, NSRCH, X, F, WORK, INCRN, IER)
END
```

```
SUBROUTINE PCN(N,X,F)
INTEGER    N,I
REAL      X(N),F
F = 0.0
DO 10 I=1,N
  F = F+X(I)**2
10 CONTINUE
RETURN
END
```

Output:

```
X = (0.0,0.0,0.0,0.0,2.0)
F = 4.0
```

***** (msl) convergence *****

IMSL IER : 0

***** parameter values *****

x(1) :	18.859	lower(1) :	0.00000E+00	upper(1) :	35.000
x(1) :	0.85926	lower(1) :	0.00000E+00	upper(1) :	10.000
	x(3) :		0.00000E+00		
	x(4) :		0.00000E+00		
	x(5) :		0.00000E+00		
	x(6) :		0.00000E+00		
	x(7) :		0.00000E+00		
	x(8) :		0.00000E+00		
	x(9) :		0.00000E+00		
	x(10) :		0.00000E+00		
	x(11) :		0.00000E+00		
	x(12) :		0.00000E+00		
	x(13) :		0.00000E+00		
	x(14) :		0.00000E+00		
	x(15) :		0.00000E+00		

AVERAGE ERROR	MAX ERROR	MIN ERROR
4.185%	18.119%	0.005%

SLT ID	SLV ID	DATA	SANGLC	% ERROR
61	98	0.99	1.00	0.91
72	98	0.99	1.00	0.57
80	98	1.00	1.00	0.97
81	100	0.99	0.99	0.61
81	100	0.97	0.99	2.29
100	72	0.91	0.95	4.83
100	80	1.03	1.00	3.43
100	100	1.00	0.114	7.89
81	123	0.99	0.99	1.40
81	100	0.93	0.99	6.64
82	123	0.99	0.99	0.30
72	123	0.71	0.76	5.87
80	123	0.99	0.99	0.43
80	123	0.99	0.99	0.99
81	123	0.99	0.99	4.95
82	123	0.84	0.99	5.50
82	123	0.81	0.99	0.74
82	123	0.84	0.99	3.44
82	123	0.91	0.91	0.91
82	123	0.95	0.91	0.51
82	123	0.93	0.91	1.97

109	133	0.99	0.93	5.74
109	142	0.69	0.75	9.04
72	80	1.09	1.04	4.97
72	80	1.09	1.03	5.17
72	80	1.07	1.03	3.62
72	80	1.06	1.03	2.82
42	126	0.99	0.97	2.48
47	126	0.87	0.85	2.07
61	126	0.97	0.97	0.46
62	126	0.98	0.98	0.31
72	126	0.94	0.90	4.31
75	126	0.93	0.91	2.32
80	126	0.97	0.98	0.58
81	126	0.98	0.97	0.55
82	126	0.98	0.97	0.97
83	126	0.99	0.99	0.02
85	126	0.99	0.98	0.75
94	126	0.92	0.94	2.01
98	126	0.98	0.99	0.56
35	133	0.81	0.81	12.11
30	133	0.80	0.89	11.70
30	133	0.82	0.93	13.88
42	133	0.85	0.87	1.85
42	133	0.83	0.85	1.92
42	133	0.84	0.85	1.60
47	133	0.74	0.71	3.64
47	133	0.73	0.71	2.63
61	133	0.87	0.87	0.22
61	133	0.86	0.86	0.38
61	133	0.88	0.88	0.55
61	133	0.88	0.88	0.88
61	133	0.87	0.87	0.48
61	133	0.86	0.87	1.38
62	133	0.82	0.89	2.16
72	133	0.75	0.75	4.28
72	133	0.75	0.76	0.88
75	133	0.77	0.78	1.85
75	133	0.71	0.78	0.61
80	133	0.88	0.88	0.12
80	133	0.88	0.88	0.68
80	133	0.88	0.88	0.72
80	133	0.89	0.89	0.64
80	133	0.88	0.88	0.28
80	133	0.88	0.88	1.85
80	133	0.88	0.91	1.41
82	133	0.91	0.91	0.37
85	133	0.88	0.88	2.44

85	133	0.91	0.90	0.66
85	133	0.92	0.90	2.02
94	133	0.79	0.81	2.39
98	133	0.93	0.91	2.12
98	133	0.90	0.91	0.68
98	133	0.89	0.91	1.95
98	133	0.90	0.90	0.41
98	133	0.91	0.91	0.03
100	133	0.93	0.93	0.15
109	133	0.92	0.93	0.91
109	133	0.92	0.93	0.72
117	133	0.95	0.95	0.18
117	133	0.94	0.95	0.68
117	133	0.94	0.95	0.55
125	133	0.96	0.96	0.11
125	133	0.95	0.96	1.08
42	135	0.88	0.83	5.62
61	135	0.87	0.84	3.79
62	135	0.90	0.85	5.16
72	135	0.76	0.72	5.85
80	135	0.88	0.86	2.59
80	135	0.84	0.85	0.90
81	135	0.78	0.86	2.80
82	135	0.88	0.85	3.59
83	135	0.94	0.88	6.32
84	135	0.97	0.90	7.18
85	135	0.91	0.87	4.53
98	135	0.89	0.88	1.24
109	135	0.91	0.90	0.81
47	136	0.87	0.84	4.77
47	136	0.88	0.84	7.34
47	136	0.88	0.84	6.08
51	136	0.83	0.79	4.34
51	136	0.82	0.79	3.61
51	136	0.82	0.80	4.14
51	136	0.82	0.80	5.85
62	136	0.82	0.80	1.88
62	136	0.85	0.81	5.96
62	136	0.84	0.81	3.56
62	136	0.88	0.82	7.68
72	136	0.73	0.68	6.54
72	136	0.74	0.68	7.79
72	136	0.72	0.68	5.27
75	136	0.75	0.71	6.84
75	136	0.75	0.71	6.86
75	136	0.77	0.71	6.29
89	136	0.88	0.82	6.88

80	136	0.87	0.82	6.18
80	136	0.89	0.82	7.32
80	136	0.87	0.82	5.87
81	136	0.88	0.82	6.48
81	136	0.85	0.81	4.18
81	136	0.86	0.82	4.84
81	136	0.86	0.82	4.88
82	136	0.88	0.81	5.72
83	136	0.87	0.84	3.77
83	136	0.89	0.84	5.39
83	136	0.90	0.84	6.81
83	136	0.92	0.85	7.84
85	136	0.89	0.83	6.78
85	136	0.88	0.83	6.08
85	136	0.89	0.83	6.83
85	136	0.92	0.84	9.10
98	136	0.91	0.85	7.08
98	136	0.90	0.84	6.18
98	136	0.92	0.85	7.71
98	136	0.92	0.84	8.40
98	136	0.90	0.84	6.84
98	136	0.82	0.84	8.20
98	136	0.91	0.84	7.88
100	136	0.95	0.84	11.18
100	136	0.97	0.85	12.87
100	136	0.84	0.84	10.40
100	136	0.97	0.89	8.22
100	136	0.92	0.87	8.28
100	136	0.97	0.81	5.75
67	136	0.57	0.60	1.88
61	136	0.73	0.73	0.47
61	136	0.78	0.73	2.82
62	136	0.76	0.74	4.88
62	136	0.73	0.75	2.46
73	136	0.82	0.82	7.13
75	136	0.81	0.85	5.86
66	136	0.73	0.75	6.10
66	136	0.80	0.76	6.82
61	136	0.78	0.78	2.33
61	136	0.77	0.78	8.87
61	136	0.83	0.78	6.28
61	136	0.78	0.78	2.84

85	138	0.82	0.77	6.57
94	138	0.59	0.68	14.61
98	138	0.73	0.79	7.87
98	138	0.83	0.78	5.51
108	138	0.89	0.83	6.44
109	138	0.74	0.82	10.35
109	138	0.85	0.81	4.24
126	138	0.89	0.86	3.02
47	142	0.49	0.51	4.08
47	142	0.49	0.51	4.27
47	142	0.51	0.51	0.05
47	142	0.50	0.51	1.84
61	142	0.59	0.67	14.08
61	142	0.63	0.65	3.64
61	142	0.63	0.66	5.53
61	142	0.66	0.66	0.51
61	142	0.62	0.66	6.18
62	142	0.67	0.67	0.07
62	142	0.63	0.67	5.76
62	142	0.62	0.67	8.44
62	142	0.64	0.68	6.20
72	142	0.51	0.55	7.54
72	142	0.53	0.55	3.50
72	142	0.49	0.55	12.13
72	142	0.53	0.55	3.58
72	142	0.54	0.55	1.53
75	142	0.57	0.57	0.32
75	142	0.55	0.57	4.08
75	142	0.56	0.57	2.27
75	142	0.55	0.57	4.33
80	142	0.67	0.69	3.01
80	142	0.68	0.68	0.12
80	142	0.68	0.69	3.79
80	142	0.68	0.68	3.59
80	142	0.61	0.68	12.08
80	142	0.61	0.70	14.20
81	142	0.64	0.68	6.74
81	142	0.64	0.69	7.54
81	142	0.65	0.68	4.45
82	142	0.68	0.71	7.02
83	142	0.69	0.70	2.14
83	142	0.67	0.71	6.36
83	142	0.61	0.72	18.12
83	142	0.67	0.70	4.85
84	142	0.76	0.73	1.41
84	142	0.73	0.74	1.23
84	142	0.73	0.73	0.63

85	142	0.67	0.70	3.83
85	142	0.68	0.70	3.13
85	142	0.67	0.69	2.92
85	142	0.68	0.69	1.81
94	142	0.54	0.60	11.37
98	142	0.67	0.71	6.28
98	142	0.67	0.72	7.83
98	142	0.70	0.72	2.47
98	142	0.70	0.71	1.98
98	142	0.72	0.71	1.42
98	142	0.71	0.71	0.65
99	142	0.69	0.71	3.27
99	142	0.69	0.71	2.79
100	142	0.72	0.71	1.11
100	142	0.72	0.72	0.60
100	142	0.74	0.71	4.19
100	142	0.69	0.74	7.61
47	144	0.46	0.45	0.89
61	144	0.62	0.61	2.35
69	144	0.62	0.62	0.20
72	144	0.47	0.50	6.44
75	144	0.50	0.52	4.78
80	144	0.61	0.63	3.64
83	144	0.64	0.65	1.98
94	144	0.50	0.55	10.24
98	144	0.63	0.66	4.83
109	144	0.65	0.69	6.28