# Prediction of Heat Capacities of Solid Inorganic Salts from Group Contributions.

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## ABSTRACT

A group contribution technique is proposed to predict the coefficients in the heat capacity correlation, $C_p = a + bT + \frac{c}{T^2} + dT^2$ , for solid inorganic salts. The results from this work are compared with fits to experimental data from the literature. It is shown to give good predictions for both simple and complex solid inorganic salts. Literature heat capacities for a large number (664) of solid inorganic salts covering a broad range of cations (129), anions (17) and ligands (2) have been used in regressions to obtain group contributions for the parameters in the heat capacity temperature function. A mean error of 3.18% is found when predicted values are compared with literature values for heat

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capacity at 298 $^{o}K$. Estimates of the error standard deviation from the regression for each additivity constant are also determined.

## INTRODUCTION

Group Contribution techniques are well studied and implemented to predict thermophysical properties such as heats of formation, $\Delta H_f^{298}$, free energies of formation, $\Delta G_f^{298}$, heat capacities, $C_p$, and liquid molar volume at normal boiling point, $V_b$, for organic compounds. Mostafa (1995) has previously described a group contribution method for predicting $\Delta H_f^{298}$ and $\Delta G_f^{298}$ of solid inorganic salts.

Read et al. (1987) describe a large number of the group contribution methods available in the literature for predicting heat capacity correlation coefficients for organic compounds. Joback (1984) used the following functional form to predict $C_p$ of organic ideal gases:

$$C_p = \left(\sum_j n_j \Delta_{a,j} - 37.93\right) + \left(\sum_j n_j \Delta_{b,j} + 0.210\right) T + \left(\sum_j n_j \Delta_{c,j} - 3.91 x 10^{-4}\right) T^2 + \left(\sum_j n_j \Delta_{d,j} + 2.06 x 10^{-7}\right) T^3 \qquad (1)$$

where, $n_j$, is the number of groups of the $j^{th}$ type, $\Delta_{k,j}$, contributions for the $k^{th}$ ( $k$=$a$, or $b$, or $c$, or $d$) coefficient and the $j^{th}$ atomic or molecular group where $T$ is in Kelvin ($^{o}K$).

Yoneda (1979) uses the same concept but a different equation for ideal gases

$$C_p = \sum_j \Delta_{a,j} + \left(\sum_j n_j \Delta_{b,j}\right)\left(\frac{T}{1000}\right) + \left(\sum_j n_j \Delta_{c,j}\right)\left(\frac{T}{1000}\right)^2 \qquad (2)$$

where, $n_j$, is the number of groups of the $j^{th}$ type, $\Delta_{k,j}$, contributions for the $k^{th}$ ( $k$=$a$, or $b$, or $c$, or $d$) coefficient and the $j^{th}$ atomic or molecular group where $T$ is in Kelvin ($^{o}K$). Thinh et at. (1976) and Benson et al. (1969) also used the same idea but different functional form of Equation 1 and 2 to predict $C_p$ for organic substances.

The following functional forms have been used by Robie et. al. (1979) to describe heat capacity of different inorganic solids.

$$C_p = a + bT + \frac{c}{T^2} + dT^2 + \frac{e}{\sqrt{T}} \tag{3}$$

$$C_p = a + bT + \frac{c}{T^2} + dT^2 \tag{4}$$

$$C_p = a + bT + \frac{c}{T^2} \tag{5}$$

$$C_p = a + bT + \frac{e}{\sqrt{T}} \tag{6}$$

$$C_p = a + bT \tag{7}$$

ASPEN PLUS™ (1990), the interactive flowsheet simulator for process modeling, developed by Aspen Technology, Inc., Cambridge, MA, uses the following functional form for the heat capacities of solids,

$$C_p = a + bT + \frac{c}{T^2} + dT^2 + \frac{f}{T} + \frac{g}{\sqrt{T^3}} \tag{8}$$

where $a$, $b$, $c$, $d$, $e$, $f$, and $g$ are constants. Kanacke and Kubaschewski (1990) used the functional form of Equation 4 for solid inorganic salts which is shown to fit experimental data well.

The inverse square of the absolute temperature functionality which appears in many of these relationship comes from Einstein's (McQuarrie, 1976) theory of the specific heat of crystals, which is

$$C_v = 3Nk\left(\frac{h\nu_E}{kT}\right)^2 \frac{e^{-h\nu_E/kT}}{\left(1-e^{-h\nu_E/kT}\right)^2} \tag{9}$$

where, $C_v$, heat capacity at constant volume, $N$, number of atoms, $k$, Boltzmann constant, $h$, Plank constant, $\nu_E$, Einstein frequency, and $T$, absolute temperature. The inverse square term appears as a dominant temperature functionality in the Taylor series expansion of Equation 9.

## DEVELOPMENT OF METHOD

In the present work the functional form of Equation 4 has been selected and written as follows,

$$C_p = \sum_j n_j \Delta_{a,j} + \left(\sum_j n_j \Delta_{b,j} x10^{-3}\right) T + \left(\sum_j n_j \Delta_{c,j}\, x10^{6}\right) \frac{1}{T^2} + \left(\sum_j n_j \Delta_{d,j}\, x10^{-6}\right) T^2 \tag{10}$$

where, $n_j$, is the number of groups of the $j^{th}$ type, $\Delta_{k,j}$, contributions for the $k^{th}$ ( $k$=$a$, or $b$, or $c$, or $d$) coefficient and the $j^{th}$ atomic or molecular group where $T$ is in Kelvin ($^oK$). The values of the group contributions are obtained by regressing on $C_p$ data from a number of (664) solid inorganic salts.

The parameters are predicted using the multiple linear regression relationship

$$\boldsymbol{b} = [\boldsymbol{X}^T\boldsymbol{X}]^{-1}\boldsymbol{X}^T\boldsymbol{y} \tag{11}$$

where $\boldsymbol{b}$ is a vector the $j^{th}$ element of which contains $\Delta_{k,j}$, the calculated prediction for the $k^{th}$ coefficient ($k$=$a$, or $b$, or $c$, or $d$) the $j^{th}$ group contributions, $\boldsymbol{X}$ is a matrix in which the element in the $i^{th}$ row and $j^{th}$ column contains $(n_{i,j} - \overline{n}_j)$, where $n_{ij}$ the number of occurrences of group $j$ in compound $i$ and $\overline{n}_j$ is the mean number of occurrences of group $j$ in all salts in the regression, and $\boldsymbol{y}$ is a vector the $i^{th}$ element of which contains the experimental values found for $C_p$, heat capacity for compound $i$. Estimates of the error in each of the calculated group contributions are obtained from the standard deviations of the parameters, $s_{\Delta j}$, which are calculated from the square roots of the diagonal elements of the variance-covariance matrix,

$$\mathbf{S} = \left(\frac{\mathbf{e}^T\,\mathbf{e}}{n-p-1}\right)\left[\mathbf{X}^T\,\mathbf{X}\right]^{-1} \tag{12}$$

where $n$ is the number of salts in the regression, $p$ is the number of group contribution parameters being estimated, and $\boldsymbol{e}$ is the error vector,

$$\boldsymbol{e} = \boldsymbol{y} - \boldsymbol{Xb} \tag{13}$$

The reader is referred to Himmelblau (1970) for a discussion of regression and statistical parameter estimation.

The data for inorganic solid salt heat capacities used in the regression are obtained from Kanacke and Kubaschewski (1990). Data for Neptunium and the hydrates are collected from Barin (1989) at different temperatures and fitted in the functional form of Equation 4

to get the coefficients *a*, *b*, *c*, and *d*. Table II gives all the groups and their contributions, $\Delta_{k,j}$, estimated by the regression for *a*, *b*, *c*, and *d*. The columns in this table list, in order, the group being estimated, the number of occurrences of that group in the regression, the contribution of that group to $\Delta_{a,j}$, the contribution of that group to $\Delta_{b,j}$, the contribution of that group to $\Delta_{c,j}$, the contribution of that group to $\Delta_{d,j}$, the standard deviations of the estimate of $\Delta_{a,j}$, the standard deviations of the estimate of $\Delta_{b,j}$, the standard deviations of the estimate of $\Delta_{c,j}$, and the standard deviations of the estimate of $\Delta_{c,j}$.

## PROCEDURE FOR PREDICTION BY THE PROPOSED METHOD

A stepwise procedure for the prediction of $C_p$ by the proposed method is described below. Table I gives an illustrative example of this sequence of calculations. The successive steps are as follows:

- Step 1: Write the molecular structural formula for the solid inorganic salt.
- Step 2: Break the molecular structural formula into appropriate ionic, atomic, or ligand molecule structural groups as given in Table II. Then calculate the numerical contributions of each group by picking the numerical value of that specific group from Table II and multiplying it by the number of occurrences of the same group in the molecular structural formula.
- Step 3: Sum of the numerical values of the various groups to yield prediction for $\sum_j n_j \Delta_{a,j}$, $\sum_j n_j \Delta_{b,j}$, $\sum_j n_j \Delta_{c,j}$, and $\sum_j n_j \Delta_{d,j}$ for Equation 10.

- Step 4: Calculated $C_p$ by plugging $\sum_j n_j \Delta_{a,j}$, $\sum_j n_j \Delta_{b,j}$, $\sum_j n_j \Delta_{c,j}$, and $\sum_j n_j \Delta_{d,j}$ in Equation 10 and using any absolute temperature $T$ ($^oK$) as required.

Dean (1979) discusses the historical Kopp's simple rule for estimating heat capacity of a liquid or solid, which states that the heat capacity of a solid inorganic compound is approximately equal to the sum of the heat capacities of the constituent elements and that an approximate value expressed in gram calories per gram formula weight can be calculated by assigning atomic heat capacities to the elements.

Table III gives a comparison of predictions of heat capacities($C_p^{298}$) for different solid inorganic salts using Kopp's rule and by the proposed method with the corresponding fits to experimental values. The columns in this table list, in order, the solid inorganic compound being considered, experimental values of heat capacity ($C_{p,Literature}^{298}$) at 298 $^oK$ found in the literature, predicted heat capacity ($C_{p,predicted}^{298}$) by the proposed method at 298 $^oK$, percent error associated with the prediction by the proposed method as compared to the experimental values, predicted heat capacity ($C_{p,predicted}^{298}$) by Kopp's rule, and percent error associated with the prediction by Kopp's rule. It can be seen that the proposed method gives better prediction. Heat capacities at the maximum temperature for which each correlation is valid (Kanacke and Kubaschewski (1990), Barin (1989)) are also predicted. A mean error of 8.17% is calculated for 649 of the 664 salts. The predictions for the reminder of the 15 compounds are poor. The errors for these poor predictions at their maxium temperature are as follows:

VO (43.53% @ 1973 $^{o}K$), $UO_2F_2$ (49.2% @ 1500 $^{o}K$), $UO_2$ (50.3% @ 2000 $^{o}K$), $TiO_2$ (46.3% @ 2130 $^{o}K$), $TiF_3$ (47.4 @ 1310 $^{o}K$), $ThO_2$ (94.5% @ 2500 $^{o}K$), $ScF_3$ (55.5 % @ 1825 $^{o}K$), $NpO_3.H_2O$ (100.4% @ 800 $^{o}K$), $MoF_3$ (93.1% @ 1237 $^{o}K$), $MoCl_3$ (52.1 % @ 926 $^{o}K$), $MoBr_3$ (60.4% @ 1082 $^{o}K$), MgO (43.8% @ 3105 $^{o}K$), $GeO_2$ (68.0% @ 1409 $^{o}K$), $FeF_3$ (46.5% @ 1132 $^{o}K$), and $Be_2SiO_4$ (63.5% @ 1806 $^{o}K$). Essentially all of these higher error levels are for oxides and helides of single cations.

## SUMMARY AND CONCLUSION

As mentioned earlier $C_p$ values predicted by the proposed method are in good agreement with the literature values at low and moderate temperatures. In Figures 1 and 2, the literature and predicted heat capacities of $CaTiO_3$ and $Fe_2(SO_4)_3$ have been plotted as a function of absolute temperatures. The temperature range used in each of the figures (Figure 1, 2, 3, & 4) are the range given by Robie et. al. (1979) over which their fit of experimental heat capacity data is said to be valid. For $CaTiO_3$, the predictions are close to experimental values up to 1200 $^{o}K$ and then the proposed method deviates by predicting higher values. For $Fe_2(SO_4)_3$, predictions are good from 300-600 $^{o}K$ and then deviates. One of the poorest predictions obtained is shown in Figure 3. Here, for $FeTiO_3$, the predictions begin to deviate at much lower temperature. Figure 4 illustrate one of cases found for under prediction at high temperature. Here, for $Mg(OH)_2$, predictions and the experimental values are almost the same from 298-600 $^{o}K$ and then the predictions deviate. In general, it can be said that the proposed method gives estimates of heat capacity with in an acceptable range of accuracy at most temperatures.

In the regression of heat capacity 664 solid inorganic salts have been used and their corresponding $C_p^{298}$ values are predicted. A mean error of 3.18%, a maximum error of 13.63% is found for these salts. This method can not be used for single metallic carbides, sulfides, hydrides, and nitrides such as $CaC_2$, CaS, $CaH_2$, and $Mg_3N_2$. This method is also not applicable for metallic solutions such as $Al_2Se_3$, ScAs, NiSe, NiTe, PbTe, etc..

**Table I. Estimation of $C_p$ from Equation 6.**

| Step Number | $C_p$ | | | | |
|---|---|---|---|---|---|
| 1 | $CaAl_2O_4$ | | | | |
| | Group | $\Delta_{a,j}$ | $\Delta_{b,j}$ | $\Delta_{c,j}$ | $\Delta_{d,j}$ |
| 2 | $Ca^{++}$ | 1(20.4698) | 1(-6.2249) | 1(-0.02629) | 1(-3.21927) |
| 2 | $Al^{+++}$ | 2(10.3059) | 2(4.5183) | 2(-0.62271) | 2(-3.7007) |
| 2 | $O^{-}$ | 4(28.1522) | 4(12.0434) | 4(-0.74718) | 4(-4.02248) |
| 3 | $\sum_j n_j \Delta_{i,j}$ | 153.6904 | 50.9853 | -4.26043 | -26.71059 |
| 4 | $C_p = \sum_j n_j \Delta_{a,j} + \left(\sum_j n_j \Delta_{b,j} x10^{-3}\right) T + \left(\sum_j n_j \Delta_{c,j} x10^{6}\right) \frac{1}{T^2} + \left(\sum_j n_j \Delta_{d,j} x10^{-6}\right) T^2$ = 153.6904 + (50.9853)x($10^{-3}$)x(298) + (-4.26043)x$10^6$/$(298)^2$ + (-26.71059)x($10^{-6}$)x$(298)^2$ = 118.54 *J/(g mol °K)*. | | | | |

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## NOMENCLATURE

$\boldsymbol{b}$ = the vector the $j^{th}$ element of which contains $\Delta_{i,j}$, the calculated estimates for the $j^{th}$ group contributions.

$C_p^{298}$ = heat capacity at 298 $^oK$, $J/(g\ mol\ ^oK)$.

$C_p$ = heat capacity, $J/(g\ mol\ ^oK)$.

$C_v$ = heat capacity at constant volume, $J/(g\ mol\ ^oK)$.

$\boldsymbol{e}$ = the vector containing the errors between the experimental values and those predicted by regression.

$h$ = Plank constant.

$k$ = Boltzmann constant.

$N$ = number of atoms.

$n$ = total number of salts in the regression.

$n_{i,j}$ = number of occurrences of group $j$ in compound $i$.

$\overline{n}_j$ = mean number of occurrences of group $j$ in all salts in the regression.

$n_j$ = number of groups of the $j^{th}$ type.

$p$ = number of group contribution parameters being estimated.

$\boldsymbol{S}$ = variance-covariance matrix.

$s_{\Delta j}$ = standard deviations of the parameters.

$V_b$ = liquid molar volume at normal boiling point.

$\boldsymbol{X}$ = the matrix the $i,j^{th}$ element of which contains $(n_{i,j} - \overline{n}_j)$.

$\boldsymbol{y}$ = the vector the $i^{th}$ element of which contains the experimental values found for $C_p$ for compound $i$.

$\nu_E$ = Einstein frequency.

$\Delta H_f^{298}$ = heat of formation, *KJ/(g mol)*.

$\Delta G_f^{298}$ = free energy of formation, *KJ/(g mol)*.

$\Delta_{k,j}$ = group contribution for *k* of $i^{th}$ ionic, atomic or ligand molecule group.

$\Delta_{a,j}$ = group contribution for *a* of $i^{th}$ ionic, atomic or ligand molecule group. *J/(g mol °K)*.

$\Delta_{b,j}$ = group contribution for *b* of $i^{th}$ ionic, atomic or ligand molecule group. $J/(g\ mol\ (°K)^2)$.

$\Delta_{c,j}$ = group contribution for *c* of $i^{th}$ ionic, atomic or ligand molecule group. *(J °K)/(g mol)*.

$\Delta_{d,j}$ = group contribution for *d* of $i^{th}$ ionic, atomic or ligand molecule group. $J/(g\ mol\ (°K)^3)$.

## LITERATURE CITED


ASPEN PLUS™. *User Guide Appendices*. 2nd edition, Aspen Technology, Inc., 1990.

Barin, Ihsan. *Thermochemical Data of Pure Substances*. VCH Verlagsgesellschaft mbH D6940 Weinheim: Germany, 1989.

Benson, S. W.; Cruickshank, F. R.; Golden, D. M.; Haugen, G. R.; O'Neal, H. E.; Rodgers, A. S.; Shaw, R.; Walsh, R. *Chem. Rev.* **1969**, 69, 279.

Dean, J. A. *Lange's Handbook of Chemistry*. McGraw-Hill Book Company: New York, 1979.

Himmelblau, D. M. *Process Analysis by Statistical Methods*. John Wiley & Sons Inc.: New York, 1970.

Joback, K. G. *Thesis. Massachusetts Institute of Technology*. Cambridge, Massachusetts, June, 1984.

Kanacke, O.; Kubaschewski, O. *Thermochemical Properties of Inorganic Substances*. Springer-Verlag: 2nd edition, Germany, 1990.

McQuarrie, D. A. *Statistical Mechanics*. Haroer & Row Publishers: New York, 1976.

Mostafa, A. T. M. G. *Predictions of Thermophysical Properties of solids from Group Contributions*. Ph.D. Dissertation. New Mexico State University, Las Cruces, New Mexico, 1995.

Read, R. C.; Prausnitz, J. M.; Poling, B. E. *The Properties of Gases and Liquids*. McGraw-Hill, Inc.: Fourth Edition, New York, 1987.

Robie, R. A.; Hemihgway, B. S.; Fisher, J. M. *Thermodynamic Properties of Minerals and Related Substances at 298.15 K and 1 Bar ($10^5$ Pascal) Pressure and at higher Temperatures*. United States Government Printing Office: Washington, 1979.

Thinh, T. P.; Trong, T. K. *Can. J. Chem. Eng.* **1976**, 54, 344.

Yoneda, Y. *Bull. Chem. Soc. Japan*. **1979**, 52, 1297.

Table II. Solid inorganic Salt Groups.
Cationic, anionic, ligand molecule groups, their contributions, number of occurrences in the regression, standard deviation ($s_{\Delta,j}$) associated with them for *a*, *b*, *c*, and *d*.

| Group | Number of Occurrences | $\Delta_{a,j}$ | $\Delta_{b,j}$ | $\Delta_{c,j}$ | $\Delta_{d,j}$ | $s_{\Delta,j}$ for $\Delta_{a,j}$ | $s_{\Delta,j}$ for $\Delta_{b,j}$ | $s_{\Delta,j}$ for $\Delta_{c,j}$ | $s_{\Delta,j}$ for $\Delta_{d,j}$ |
|---|---|---|---|---|---|---|---|---|---|
| **Cations** | | | | | | | | | |
| $Ag^{+}$ | 8 | 11.398 | 24.063 | 0.434 | 2.106 | 5.613 | 12.287 | 0.269 | 8.322 |
| $Al^{+++}$ | 81 | 10.306 | 4.518 | -0.623 | -3.701 | 3.420 | 7.485 | 0.164 | 5.069 |
| $As^{+++}$ | 6 | -18.849 | 69.121 | 0.995 | 6.034 | 5.785 | 12.663 | 0.277 | 8.576 |
| $As^{+++++}$ | 4 | -16.941 | 25.671 | 1.183 | 5.796 | 2.715 | 5.943 | 0.130 | 4.025 |
| $B^{+++}$ | 59 | -13.188 | 16.765 | 0.273 | -0.219 | 14.813 | 32.424 | 0.710 | 21.960 |
| $Ba^{++}$ | 23 | 26.676 | -15.773 | 0.054 | 7.523 | 1.546 | 3.384 | 0.074 | 2.292 |
| $Be^{++}$ | 16 | -5.164 | 22.314 | -0.002 | 6.544 | 2.783 | 6.092 | 0.133 | 4.126 |
| $Bi^{+++}$ | 9 | -3.363 | 14.344 | 1.658 | 2.171 | 1.257 | 2.753 | 0.060 | 1.864 |
| $Ca^{++}$ | 64 | 20.470 | -6.225 | -0.026 | -3.219 | 2.384 | 5.217 | 0.114 | 3.534 |
| $Cd^{++}$ | 14 | 21.910 | -23.495 | 0.561 | 6.178 | 4.737 | 10.369 | 0.227 | 7.023 |
| $Ce^{+++}$ | 9 | 13.011 | -7.089 | 0.762 | 4.687 | 3.088 | 6.760 | 0.148 | 4.579 |
| $Ce^{++++}$ | 1 | 8.506 | -6.387 | 0.734 | 8.045 | 3.010 | 6.589 | 0.144 | 4.462 |
| $Cm^{+++}$ | 1 | -5.346 | 10.658 | 0.076 | -3.166 | 6.906 | 15.116 | 0.331 | 10.238 |
| $Co^{++}$ | 17 | 26.552 | -19.272 | 0.327 | 5.245 | 18.490 | 40.473 | 0.887 | 27.411 |
| $Co^{+++}$ | 1 | 34.158 | -42.075 | -0.149 | -4.614 | 12.259 | 26.834 | 0.588 | 18.174 |
| $Cr^{++}$ | 4 | 16.779 | -8.351 | 0.152 | 0.073 | 1.353 | 2.962 | 0.065 | 2.006 |
| $Cr^{+++}$ | 22 | 21.086 | -16.392 | 0.067 | 5.298 | 3.272 | 7.162 | 0.157 | 4.851 |
| $Cr^{++++++}$ | 4 | -23.112 | 27.266 | 1.662 | 8.719 | 3.228 | 7.066 | 0.155 | 4.786 |
| $Cs^{+}$ | 8 | 20.779 | -0.058 | 0.520 | 11.137 | 10.108 | 22.126 | 0.485 | 14.985 |
| $Cu^{+}$ | 7 | 11.289 | 12.683 | 0.270 | 4.246 | 13.191 | 28.874 | 0.633 | 19.555 |

| Group | Number of Occurrences | $\Delta_{a,j}$ | $\Delta_{b,j}$ | $\Delta_{c,j}$ | $\Delta_{d,j}$ | $s_{\Delta,j}$ for $\Delta_{a,j}$ | $s_{\Delta,j}$ for $\Delta_{b,j}$ | $s_{\Delta,j}$ for $\Delta_{c,j}$ | $s_{\Delta,j}$ for $\Delta_{d,j}$ |
|---|---|---|---|---|---|---|---|---|---|
| $Cu^{++}$ | 11 | 19.179 | 3.018 | -0.002 | -1.275 | 9.051 | 19.811 | 0.434 | 13.418 |
| $Dy^{+++}$ | 4 | 21.060 | -15.320 | 0.476 | 2.925 | 5.094 | 11.151 | 0.244 | 7.552 |
| $Er^{+++}$ | 2 | 17.635 | -17.241 | 1.542 | -3.292 | 13.191 | 28.874 | 0.633 | 19.555 |
| $Eu^{++}$ | 2 | 22.957 | -9.764 | 0.500 | 3.050 | 11.995 | 26.256 | 0.575 | 17.782 |
| $Eu^{+++}$ | 6 | 35.717 | -36.906 | 0.298 | 18.834 | 15.374 | 33.652 | 0.737 | 22.791 |
| $Fe^{++}$ | 15 | 20.486 | -5.415 | 0.055 | 5.393 | 6.074 | 13.295 | 0.291 | 9.004 |
| $Fe^{+++}$ | 26 | 16.618 | 3.328 | 0.082 | 5.002 | 13.171 | 28.830 | 0.632 | 19.525 |
| $Ga^{+++}$ | 9 | 16.577 | -11.146 | -0.034 | 5.207 | 4.675 | 10.233 | 0.224 | 6.930 |
| $Gd^{+++}$ | 7 | 20.474 | -20.495 | 0.163 | 3.088 | 14.364 | 31.441 | 0.689 | 21.294 |
| $Ge^{++}$ | 2 | 17.815 | -5.864 | 0.556 | 3.312 | 6.528 | 14.289 | 0.313 | 9.678 |
| $Ge^{++++}$ | 2 | -7.106 | 41.113 | 0.226 | 6.623 | 9.494 | 20.782 | 0.455 | 14.075 |
| $H^{+}$ | 12 | -5.217 | 25.754 | 0.232 | 2.576 | 6.839 | 14.969 | 0.328 | 10.138 |
| $Hf^{++}$ | 1 | 8.841 | -27.084 | 0.280 | 2.601 | 4.451 | 9.744 | 0.213 | 6.599 |
| $Hf^{++++}$ | 9 | 20.580 | -22.025 | -0.050 | 2.633 | 6.366 | 13.935 | 0.305 | 9.438 |
| $Hg^{+}$ | 8 | 23.601 | 0.155 | 0.078 | 0.036 | 25.914 | 56.722 | 1.243 | 38.416 |
| $Hg^{++}$ | 6 | 8.228 | 19.740 | 0.585 | 2.319 | 2.770 | 6.063 | 0.133 | 4.106 |
| $Ho^{+++}$ | 6 | 33.919 | -49.884 | 0.133 | 19.321 | 6.964 | 15.244 | 0.334 | 10.324 |
| $In^{+}$ | 3 | 15.693 | 13.602 | 0.212 | 0.561 | 7.036 | 15.401 | 0.337 | 10.430 |
| $In^{++}$ | 1 | 5.362 | 29.459 | 0.502 | -1.314 | 7.587 | 16.607 | 0.364 | 11.247 |
| $In^{+++}$ | 5 | 13.433 | -4.548 | 0.310 | 2.953 | 7.675 | 16.800 | 0.368 | 11.378 |
| $Ir^{+++}$ | 2 | 13.108 | -18.124 | 0.469 | 0.573 | 5.394 | 11.808 | 0.259 | 7.997 |
| $Ir^{++++}$ | 1 | 5.576 | -3.667 | 0.394 | 8.045 | 6.983 | 15.285 | 0.335 | 10.352 |
| $K^{+}$ | 48 | 25.309 | -2.284 | 0.218 | 5.174 | 18.426 | 40.333 | 0.884 | 27.316 |
| $La^{+++}$ | 8 | 15.803 | -11.296 | 0.458 | 3.344 | 18.643 | 40.808 | 0.894 | 27.638 |
| $Li^{+}$ | 47 | 15.639 | 4.124 | -0.007 | 7.973 | 6.207 | 13.585 | 0.298 | 9.201 |
| $Lu^{+++}$ | 3 | 18.605 | -16.153 | 0.172 | 3.904 | 10.230 | 22.392 | 0.491 | 15.166 |

| Group | Number of Occurrences | $\Delta_{a,j}$ | $\Delta_{b,j}$ | $\Delta_{c,j}$ | $\Delta_{d,j}$ | $s_{\Delta,j}$ for $\Delta_{a,j}$ | $s_{\Delta,j}$ for $\Delta_{b,j}$ | $s_{\Delta,j}$ for $\Delta_{c,j}$ | $s_{\Delta,j}$ for $\Delta_{d,j}$ |
|---|---|---|---|---|---|---|---|---|---|
| $Mg^{++}$ | 32 | 14.639 | -0.637 | -0.074 | -0.609 | 11.283 | 24.698 | 0.541 | 16.727 |
| $Mn^{++}$ | 15 | 21.419 | -15.908 | 0.265 | 5.652 | 13.410 | 29.352 | 0.643 | 19.879 |
| $Mn^{+++}$ | 4 | 8.913 | 3.070 | 0.454 | 5.448 | 19.073 | 41.749 | 0.915 | 28.275 |
| $Mo^{++}$ | 3 | 22.549 | -9.633 | 0.289 | 1.122 | 1.575 | 3.447 | 0.076 | 2.335 |
| $Mo^{+++}$ | 4 | -28.076 | 84.735 | 1.976 | 0.108 | 5.333 | 11.673 | 0.256 | 7.906 |
| $Mo^{++++}$ | 3 | 19.349 | -24.670 | 0.62 | 0.855 | 6.632 | 14.516 | 0.318 | 9.831 |
| $Mo^{+++++}$ | 2 | -48.550 | 202.730 | 1.237 | -5.487 | 25.970 | 56.846 | 1.245 | 38.500 |
| $Mo^{++++++}$ | 11 | -7.473 | -7.423 | 1.279 | 13.430 | 10.108 | 22.125 | 0.485 | 14.985 |
| $Na^{+}$ | 91 | 14.186 | 9.665 | 0.529 | 4.851 | 13.171 | 28.830 | 0.632 | 19.526 |
| $Nb^{+++}$ | 1 | 20.593 | -14.387 | 0.043 | -1.971 | 13.265 | 29.036 | 0.636 | 19.665 |
| $Nb^{++++}$ | 3 | 12.016 | -14.823 | 0.494 | 2.709 | 7.278 | 15.931 | 0.349 | 10.789 |
| $Nb^{+++++}$ | 5 | 19.843 | -33.720 | 0.517 | 1.065 | 25.907 | 56.707 | 1.242 | 38.406 |
| $Nd^{+++}$ | 9 | 15.042 | -4.286 | 0.450 | 3.311 | 15.349 | 33.597 | 0.736 | 22.754 |
| $NH4^{+}$ | 4 | 4.205 | 116.120 | 1.206 | 2.166 | 10.477 | 22.932 | 0.502 | 15.531 |
| $Ni^{++}$ | 14 | 22.497 | -6.671 | -0.022 | 6.234 | 15.110 | 33.074 | 0.725 | 22.400 |
| $Np^{+++}$ | 2 | 23.683 | -10.822 | 0.742 | -3.274 | 13.265 | 29.036 | 0.636 | 19.665 |
| $Np^{++++}$ | 3 | -12.661 | 62.760 | 1.250 | -48.715 | 15.378 | 33.662 | 0.737 | 22.798 |
| $Np^{++++++}$ | 2 | -19.545 | -43.129 | 1.616 | 356.929 | 18.835 | 41.228 | 0.903 | 27.922 |
| $P^{+++++}$ | 12 | -39.486 | 50.248 | 1.686 | 2.325 | 8.664 | 18.965 | 0.415 | 12.844 |
| $Pb^{++}$ | 26 | 14.632 | 7.448 | 0.642 | 4.828 | 25.970 | 56.846 | 1.245 | 38.500 |
| $Pb^{++++}$ | 1 | 0.7457 | 4.913 | 1.076 | 8.045 | 26.165 | 57.272 | 1.255 | 38.789 |
| $Pd^{++}$ | 3 | 15.727 | -2.973 | 0.496 | 1.895 | 25.907 | 56.707 | 1.242 | 38.406 |
| $Pr^{+++}$ | 6 | 20.343 | -11.940 | 0.213 | 2.084 | 25.970 | 56.846 | 1.245 | 38.500 |
| $Pr^{++++}$ | 1 | 21.266 | 0.933 | 0.419 | 8.045 | 10.836 | 23.719 | 0.520 | 16.064 |
| $Pt^{++}$ | 2 | 14.033 | 4.772 | 0.453 | 0.382 | 15.136 | 33.131 | 0.726 | 22.439 |
| $Pt^{+++}$ | 2 | 28.058 | -25.164 | 0.679 | 0.573 | 7.393 | 16.183 | 0.355 | 10.960 |

| Group | Number of Occurrences | $\Delta_{a,j}$ | $\Delta_{b,j}$ | $\Delta_{c,j}$ | $\Delta_{d,j}$ | $s_{\Delta,j}$ for $\Delta_{a,j}$ | $s_{\Delta,j}$ for $\Delta_{b,j}$ | $s_{\Delta,j}$ for $\Delta_{c,j}$ | $s_{\Delta,j}$ for $\Delta_{d,j}$ |
|---|---|---|---|---|---|---|---|---|---|
| $Pt^{++++}$ | 2 | 43.127 | -50.286 | 0.905 | 0.764 | 7.690 | 16.832 | 0.369 | 11.400 |
| $Pu^{+++}$ | 7 | 31.509 | -15.262 | 0.127 | 3.352 | 10.108 | 22.126 | 0.485 | 14.985 |
| $Pu^{++++}$ | 2 | 35.028 | -39.982 | -0.268 | -1.420 | 25.819 | 56.515 | 1.238 | 38.276 |
| $Pu^{++++++}$ | 2 | -17.410 | 43.930 | 0.385 | -1.932 | 15.111 | 33.076 | 0.725 | 22.402 |
| $Rb^{+}$ | 16 | 19.747 | 5.160 | 0.526 | 7.198 | 10.959 | 23.987 | 0.526 | 16.246 |
| $Re^{++++}$ | 1 | 11.056 | -11.407 | 0.201 | 8.045 | 25.970 | 56.846 | 1.245 | 38.500 |
| $Re^{+++++}$ | 1 | 3.204 | -19.960 | 0.492 | 12.067 | 9.768 | 21.382 | 0.468 | 14.481 |
| $Re^{+++++++}$ | 2 | -7.326 | 6.207 | 1.683 | 15.007 | 18.569 | 40.645 | 0.890 | 27.528 |
| $Rh^{+++}$ | 4 | 10.964 | 3.8319 | 0.338 | 4.214 | 1.660 | 3.634 | 0.080 | 2.461 |
| $Ru^{+++}$ | 1 | 35.233 | -31.127 | 0.754 | -1.971 | 6.705 | 14.676 | 0.322 | 9.940 |
| $Ru^{++++}$ | 1 | 20.326 | -13.287 | -0.920 | 8.045 | 5.090 | 11.141 | 0.244 | 7.545 |
| $Sb^{+++}$ | 6 | -11.375 | 36.678 | 1.780 | 0.090 | 6.772 | 14.823 | 0.325 | 10.039 |
| $Sc^{+++}$ | 5 | 12.644 | -15.208 | 0.330 | 2.953 | 6.171 | 13.507 | 0.296 | 9.148 |
| $Se^{++++}$ | 6 | -14.644 | 16.581 | 1.731 | 5.589 | 18.623 | 40.763 | 0.893 | 27.607 |
| $Se^{+++++}$ | 2 | 0.120 | -8.773 | 0.697 | 10.056 | 8.016 | 17.547 | 0.384 | 11.884 |
| $Se^{++++++}$ | 2 | -63.818 | 110.803 | 2.335 | 10.990 | 18.623 | 40.763 | 0.893 | 27.607 |
| $Si^{++++}$ | 79 | -2.308 | 4.382 | -0.041 | -3.301 | 7.003 | 15.329 | 0.336 | 10.382 |
| $Sm^{++}$ | 1 | 24.182 | -4.011 | 0.502 | -1.314 | 6.803 | 14.892 | 0.326 | 10.086 |
| $Sm^{+++}$ | 8 | 22.693 | -10.606 | 0.327 | 3.826 | 18.411 | 40.299 | 0.883 | 27.294 |
| $Sn^{++}$ | 6 | 16.189 | 5.634 | 0.378 | 1.586 | 7.268 | 15.908 | 0.349 | 10.774 |
| $Sn^{++++}$ | 1 | 10.166 | -7.447 | -0.180 | 8.045 | 13.249 | 29.000 | 0.635 | 19.641 |
| $Sr^{++}$ | 14 | 15.410 | -0.275 | 0.381 | 4.159 | 6.889 | 15.079 | 0.330 | 10.213 |
| $Sr^{++++}$ | 1 | 17.666 | -6.047 | 1.494 | 8.045 | 7.441 | 16.287 | 0.357 | 11.030 |
| $Ta^{+++}$ | 1 | 16.373 | -14.807 | 0.043 | -1.971 | 18.623 | 40.763 | 0.893 | 27.607 |
| $Ta^{++++}$ | 1 | 27.033 | -41.503 | -0.208 | -2.628 | 7.932 | 17.361 | 0.380 | 11.758 |
| $Ta^{+++++}$ | 9 | 12.959 | -20.800 | 0.439 | 4.567 | 7.475 | 16.363 | 0.358 | 11.082 |

| Group | Number of Occurrences | $\Delta_{a,j}$ | $\Delta_{b,j}$ | $\Delta_{c,j}$ | $\Delta_{d,j}$ | $s_{\Delta,j}$ for $\Delta_{a,j}$ | $s_{\Delta,j}$ for $\Delta_{b,j}$ | $s_{\Delta,j}$ for $\Delta_{c,j}$ | $s_{\Delta,j}$ for $\Delta_{d,j}$ |
|---|---|---|---|---|---|---|---|---|---|
| $Tb^{+++}$ | 5 | 18.899 | -10.177 | 0.342 | 3.065 | 15.232 | 33.340 | 0.730 | 22.580 |
| $Tb^{++++}$ | 1 | 8.506 | -6.387 | 0.733 | 8.045 | 8.228 | 18.010 | 0.395 | 12.198 |
| $Tc^{++++}$ | 1 | 12.316 | -12.577 | 0.038 | 8.045 | 25.819 | 56.515 | 1.238 | 38.276 |
| $Tc^{++++++}$ | 1 | 23.493 | -36.130 | 2.242 | 12.067 | 7.932 | 17.361 | 0.380 | 11.758 |
| $Te^{++++}$ | 2 | 20.470 | -25.515 | 0.999 | 2.709 | 18.411 | 40.299 | 0.883 | 27.294 |
| $Th^{++++}$ | 11 | 20.291 | -28.458 | 0.351 | -1.633 | 8.577 | 18.773 | 0.411 | 12.715 |
| $Ti^{++}$ | 4 | 21.321 | -9.603 | 0.209 | 1.847 | 25.871 | 56.630 | 1.241 | 38.353 |
| $Ti^{+++}$ | 7 | 0.689 | 23.784 | 0.839 | 3.471 | 8.857 | 19.388 | 0.425 | 13.131 |
| $Ti^{++++}$ | 34 | 10.043 | -7.562 | 0.299 | 11.414 | 25.907 | 56.707 | 1.242 | 38.406 |
| $Tl^{+}$ | 7 | 15.850 | 20.050 | 0.507 | 0.635 | 26.065 | 57.054 | 1.250 | 38.641 |
| $Tl^{+++}$ | 3 | 25.172 | -13.439 | -0.203 | 5.087 | 8.112 | 17.756 | 0.389 | 12.025 |
| $Tm^{+++}$ | 4 | 23.189 | -19.727 | 0.482 | 3.370 | 18.959 | 41.499 | 0.909 | 28.106 |
| $U^{+++}$ | 4 | 17.864 | -10.375 | 0.780 | 0.108 | 18.569 | 40.645 | 0.890 | 27.528 |
| $U^{++++}$ | 7 | 26.669 | -29.923 | -0.066 | 2.171 | 25.819 | 56.515 | 1.238 | 38.276 |
| $U^{+++++}$ | 4 | 13.890 | -31.178 | 0.627 | -2.126 | 19.886 | 43.528 | 0.954 | 29.480 |
| $U^{++++++}$ | 11 | -14.769 | 50.875 | 1.654 | -14.399 | 26.165 | 57.272 | 1.255 | 38.789 |
| $V^{++}$ | 4 | 20.124 | -11.173 | 0.087 | 1.847 | 25.970 | 56.846 | 1.245 | 38.500 |
| $V^{+++}$ | 4 | 20.671 | -27.881 | 0.199 | 0.867 | 25.970 | 56.846 | 1.245 | 38.500 |
| $V^{++++}$ | 3 | 2.121 | 2.604 | 1.214 | 1.988 | 18.487 | 40.466 | 0.887 | 27.407 |
| $V^{+++++}$ | 20 | -1.279 | -5.243 | 0.697 | 13.608 | 18.386 | 40.246 | 0.882 | 27.257 |
| $W^{++}$ | 1 | 18.062 | 1.149 | 0.502 | -1.314 | 18.487 | 40.466 | 0.887 | 27.407 |
| $W^{++++}$ | 2 | 6.405 | 3.023 | 0.790 | 2.709 | 18.679 | 40.886 | 0.896 | 27.691 |
| $W^{+++++}$ | 2 | -6.784 | 42.333 | 1.062 | 0.956 | 6.585 | 14.415 | 0.316 | 9.763 |
| $W^{++++++}$ | 20 | -23.788 | 35.451 | 1.836 | 9.893 | 11.045 | 24.177 | 0.530 | 16.374 |
| $Y^{+++}$ | 5 | 22.197 | -22.411 | 0.002 | 3.065 | 3.823 | 8.368 | 0.183 | 5.667 |
| $Yb^{++}$ | 1 | 14.772 | 0.169 | 0.502 | -1.314 | 25.970 | 56.846 | 1.245 | 38.500 |

| Group | Number of Occurrences | $\Delta_{a,j}$ | $\Delta_{b,j}$ | $\Delta_{c,j}$ | $\Delta_{d,j}$ | $s_{\Delta,j}$ for $\Delta_{a,j}$ | $s_{\Delta,j}$ for $\Delta_{b,j}$ | $s_{\Delta,j}$ for $\Delta_{c,j}$ | $s_{\Delta,j}$ for $\Delta_{d,j}$ |
|---|---|---|---|---|---|---|---|---|---|
| $Yb^{+++}$ | 4 | 23.895 | -21.427 | 0.346 | 2.925 | 7.762 | 16.991 | 0.372 | 11.507 |
| $Zn^{++}$ | 18 | 12.599 | -0.744 | 0.377 | 4.203 | 12.729 | 27.863 | 0.610 | 18.871 |
| $Zr^{++}$ | 4 | 30.330 | -18.041 | 0.077 | 0.072 | 8.019 | 17.554 | 0.385 | 11.888 |
| $Zr^{+++}$ | 4 | 26.864 | -34.755 | -0.144 | 0.108 | 11.751 | 25.722 | 0.564 | 17.421 |
| $Zr^{++++}$ | 13 | 17.188 | -23.478 | -0.063 | 7.098 | 7.905 | 17.304 | 0.379 | 11.720 |
| **Anions** | | | | | | | | | |
| $Br^-$ | 166 | 26.093 | 14.767 | -0.201 | -1.039 | 9.698 | 21.228 | 0.465 | 14.377 |
| $Cl^-$ | 295 | 26.609 | 10.376 | -0.251 | 0.657 | 8.392 | 18.368 | 0.402 | 12.440 |
| $ClO3^-$ | 2 | 56.325 | 104.045 | -1.043 | -5.013 | 11.537 | 25.253 | 0.553 | 17.103 |
| $ClO4^-$ | 4 | 113.901 | 46.380 | -3.511 | -6.944 | 8.502 | 18.611 | 0.408 | 12.605 |
| $CO3^{--}$ | 15 | 47.278 | 86.757 | -0.887 | -5.133 | 18.462 | 40.411 | 0.885 | 27.369 |
| $F^-$ | 247 | 22.041 | 15.652 | -0.244 | 1.538 | 15.349 | 33.597 | 0.736 | 22.754 |
| $HCO3^-$ | 2 | 26.758 | 138.905 | -0.373 | -5.013 | 18.958 | 41.497 | 0.909 | 28.105 |
| $I^-$ | 132 | 26.999 | 13.542 | -0.182 | -1.300 | 7.373 | 16.138 | 0.354 | 10.930 |
| $N^{---}$ | 2 | 24.083 | 31.806 | -0.764 | 3.644 | 15.410 | 33.732 | 0.739 | 22.845 |
| $NO2^-$ | 1 | 18.307 | 126.388 | 0.596 | -4.044 | 19.692 | 43.103 | 0.944 | 29.192 |
| $NO3^-$ | 120 | 49.766 | 83.928 | -0.478 | -7.040 | 26.387 | 57.758 | 1.265 | 39.118 |
| $O^-$ | 36 | 34.706 | 3.050 | -1.052 | -6.604 | 4.844 | 10.604 | 0.232 | 7.182 |
| $O^{--}$ | 1155 | 28.152 | 12.043 | -0.747 | -4.023 | 18.490 | 40.473 | 0.887 | 27.411 |
| $OH^-$ | 16 | 28.917 | 30.730 | -0.628 | 3.257 | 4.780 | 10.462 | 0.229 | 7.086 |
| $PO4^{---}$ | 6 | 95.827 | 56.863 | -2.462 | -7.691 | 26.695 | 58.433 | 1.280 | 39.575 |
| $SO3^{--}$ | 1 | 78.739 | 24.184 | -1.058 | -9.702 | 11.282 | 24.694 | 0.541 | 16.725 |
| $SO4^{--}$ | 49 | 85.866 | 52.357 | -1.925 | -0.047 | 2.270 | 4.969 | 0.109 | 3.365 |
| **Ligand Molecules** | | | | | | | | | |

| Group | Number of Occurrences | $\Delta_{a,j}$ | $\Delta_{b,j}$ | $\Delta_{c,j}$ | $\Delta_{d,j}$ | $s_{\Delta,j}$ for $\Delta_{a,j}$ | $s_{\Delta,j}$ for $\Delta_{b,j}$ | $s_{\Delta,j}$ for $\Delta_{c,j}$ | $s_{\Delta,j}$ for $\Delta_{d,j}$ |
|---|---|---|---|---|---|---|---|---|---|
| CO | 18 | 36.332 | 20.257 | -0.265 | -1.780 | 26.181 | 57.306 | 1.256 | 38.812 |
| H2O | 39 | 15.458 | 66.593 | 0.470 | -40.518 | 3.561 | 7.794 | 0.171 | 5.278 |

Table III. Predicted and Experimental Values, Percent Error.
Comparision of heat capacities by the proposed method, Kopp's rule with the corresponding experimental values and the percent errors (% Error) associated with some selected solid inorganic salts.

| COMPOUND | $C_{p,Literature}^{298}$ | $C_{p,predicted}^{298}$ Proposed Method | % Error Proposed Method | $C_{p,predicted}^{298}$ Kopp's Rule | % Error Kopp's Rule |
|---|---|---|---|---|---|
| $Ag_2CO_3$ | 111.60 | 109.98 | 1.45 | 109.62 | 1.77 |
| $Ag_2SO_4$ | 131.44 | 127.08 | 3.31 | 141.42 | 7.59 |
| $AgNO_2$ | 81.34 | 85.97 | 5.70 | 85.35 | 4.94 |
| $AgNO_3$ | 93.01 | 92.41 | 0.64 | 102.09 | 9.76 |
| $Al(OH)_3$ | 93.05 | 98.19 | 5.53 | 105.02 | 12.87 |
| $Al_2(SO_4)_3$ | 260.15 | 248.00 | 4.67 | 320.49 | 23.20 |
| AlOCl | 56.83 | 54.21 | 4.61 | 68.62 | 20.74 |
| $AlPO_4$ | 92.98 | 88.67 | 4.63 | 115.48 | 24.19 |
| $Ba(NO_3)_2$ | 151.32 | 160.79 | 6.25 | 178.24 | 17.79 |
| $Ba_2TiO_4$ | 149.13 | 150.56 | 0.95 | 144.77 | 2.93 |
| $Ba_3Al_2O_6$ | 215.35 | 216.20 | 0.39 | 230.12 | 6.86 |
| $BaCO_3$ | 87.97 | 85.94 | 2.31 | 83.68 | 4.88 |
| $BaHfO_3$ | 108.25 | 105.86 | 2.21 | 102.09 | 5.69 |
| $BaSO_4$ | 101.67 | 103.04 | 1.35 | 115.48 | 13.58 |
| $BaTiO_3$ | 102.38 | 104.34 | 1.91 | 102.09 | 0.29 |
| $BaV_2O_6$ | 172.78 | 173.51 | 0.42 | 178.24 | 3.16 |
| $BaZrO_3$ | 105.39 | 102.27 | 2.95 | 102.09 | 3.13 |
| $Be(OH)_2$ | 65.55 | 64.63 | 1.40 | 78.66 | 20.01 |
| $BeAl_2O_4$ | 104.88 | 102.55 | 2.22 | 144.77 | 38.03 |
| $BeAl_6O_{10}$ | 261.81 | 257.61 | 1.60 | 348.95 | 33.28 |
| $BeSO_4$ | 85.60 | 81.84 | 4.40 | 115.48 | 34.90 |
| $Bi_2(SO_4)_3$ | 278.82 | 278.93 | 0.04 | 320.49 | 14.95 |
| BiOCl | 70.16 | 69.67 | 0.70 | 68.62 | 2.20 |
| $Ca(NO_3)_2$ | 149.29 | 155.57 | 4.20 | 178.24 | 19.39 |
| $Ca(OH)_2$ | 87.56 | 80.62 | 7.92 | 78.66 | 10.16 |
| $Ca_2B_2O_5$ | 147.05 | 140.63 | 4.37 | 158.16 | 7.55 |
| $Ca_2P_2O_7$ | 187.70 | 186.21 | 0.79 | 214.22 | 14.13 |
| $Ca_2V_2O_7$ | 213.88 | 209.29 | 2.15 | 220.92 | 3.29 |
| $Ca_3Al_2O_6$ | 209.65 | 200.54 | 4.34 | 230.12 | 9.76 |
| $Ca_3B_2O_6$ | 187.77 | 181.63 | 3.27 | 200.83 | 6.96 |
| $Ca_3P_2O8$ | 236.03 | 227.22 | 3.73 | 256.90 | 8.84 |
| $Ca_3WO_6$ | 202.24 | 200.25 | 0.99 | 204.18 | 0.96 |
| $CaAl_2O_4$ | 120.55 | 118.54 | 1.67 | 144.77 | 20.08 |
| $CaAl_4O_7$ | 193.83 | 196.07 | 1.16 | 246.86 | 27.36 |
| $CaB_2O_4$ | 103.83 | 99.63 | 4.05 | 115.48 | 11.22 |
| $CaB_4O_7$ | 157.74 | 158.25 | 0.33 | 188.28 | 19.36 |

| COMPOUND | $C_{p,Literature}^{298}$ | $C_{p,predicted}^{298}$ Proposed Method | % Error Proposed Method | $C_{p,predicted}^{298}$ Kopp's Rule | % Error Kopp's Rule |
|---|---|---|---|---|---|
| $CaCO_3.MgCO_3$ | 155.18 | 156.98 | 1.16 | 167.36 | 7.85 |
| $CaCr_2O_4$ | 146.59 | 144.77 | 1.24 | 144.77 | 1.24 |
| $CaFe_2O_5$ | 194.05 | 188.88 | 2.66 | 187.44 | 3.40 |
| $CaMgO_2$ | 79.61 | 77.54 | 2.60 | 85.35 | 7.22 |
| $CaMoO_4$ | 117.06 | 115.82 | 1.06 | 118.83 | 1.51 |
| $CaO.HfO_2$ | 105.71 | 100.64 | 4.80 | 102.09 | 3.42 |
| $CaUO_4$ | 130.44 | 127.65 | 2.13 | 118.83 | 8.90 |
| $CaV_2O_6$ | 170.74 | 168.29 | 1.44 | 178.24 | 4.39 |
| $Li_2B_4O_7$ | 170.34 | 175.21 | 2.86 | 214.22 | 25.76 |
| $Li_2BeF_4$ | 134.97 | 133.42 | 1.15 | 161.50 | 19.66 |
| $Li_2CO_3$ | 97.96 | 97.68 | 0.30 | 109.62 | 11.90 |
| $Li_2HfO_3$ | 111.87 | 117.59 | 5.11 | 128.03 | 14.44 |
| $Li_2Nb_2O_6$ | 198.55 | 204.22 | 2.86 | 204.18 | 2.83 |
| $Li_2SO_4$ | 117.14 | 114.78 | 2.01 | 141.42 | 20.73 |
| $Li_2Ta_2O_6$ | 200.14 | 197.02 | 1.56 | 204.18 | 2.02 |
| $Li_2WO_4$ | 133.34 | 135.20 | 1.39 | 144.77 | 8.57 |
| $Li_2ZrO_3$ | 110.20 | 114.01 | 3.45 | 128.03 | 16.18 |
| $Li_3AlF_6$ | 202.30 | 201.38 | 0.45 | 229.28 | 13.34 |
| $LiBeF_3$ | 92.61 | 91.83 | 0.84 | 114.64 | 23.79 |
| $LiClO_4$ | 104.94 | 105.06 | 0.12 | 118.83 | 13.24 |
| $LiNO_3$ | 89.11 | 86.26 | 3.20 | 102.09 | 14.56 |
| LiOH | 49.75 | 48.79 | 1.93 | 52.30 | 5.13 |
| $Mg(NO_3)_2$ | 141.90 | 151.10 | 6.48 | 178.24 | 25.61 |
| $Mg(OH)_2$ | 77.49 | 76.15 | 1.73 | 78.66 | 1.50 |
| $Mg_2V_2O_7$ | 202.26 | 200.35 | 0.94 | 220.92 | 9.23 |
| $Mg_3P_2O_8$ | 213.09 | 213.82 | 0.34 | 256.90 | 20.56 |
| $MgAl_2O_4$ | 115.94 | 114.07 | 1.61 | 144.77 | 24.87 |
| $MgCO_3$ | 75.40 | 76.26 | 1.13 | 83.68 | 10.98 |
| $MgFe_2O_4$ | 137.76 | 143.41 | 4.10 | 144.77 | 5.09 |
| $MgMoO_4$ | 110.88 | 111.35 | 0.42 | 118.83 | 7.16 |
| $MgSO_4$ | 95.57 | 93.36 | 2.31 | 115.48 | 20.83 |
| $MgTi_2O_5$ | 146.60 | 152.76 | 4.21 | 161.50 | 10.17 |
| $MgTiO_3$ | 91.17 | 94.65 | 3.82 | 102.09 | 11.98 |
| $MgV_2O_6$ | 159.87 | 163.82 | 2.47 | 178.24 | 11.49 |
| $MgWO_4$ | 109.83 | 113.78 | 3.59 | 118.83 | 8.19 |
| $UBr_3$ | 108.73 | 107.96 | 0.71 | 103.76 | 4.57 |
| $UBr_4$ | 128.11 | 129.74 | 1.27 | 129.70 | 1.24 |
| $UCl_3$ | 102.52 | 104.35 | 1.79 | 103.76 | 1.21 |
| $UCl_4$ | 120.77 | 124.93 | 3.44 | 129.70 | 7.40 |
| $UCl_5$ | 144.57 | 146.12 | 1.08 | 155.64 | 7.66 |

| COMPOUND | $C_{p,Literature}^{298}$ | $C_{p,predicted}^{298}$ Proposed Method | % Error Proposed Method | $C_{p,predicted}^{298}$ Kopp's Rule | % Error Kopp's Rule |
|---|---|---|---|---|---|
| $UCl_6$ | 175.53 | 179.32 | 2.16 | 181.59 | 3.45 |
| $UF_3$ | 95.08 | 95.86 | 0.82 | 88.70 | 6.71 |
| $UF_4$ | 116.01 | 113.60 | 2.08 | 109.62 | 5.51 |
| $UF_5$ | 132.30 | 131.96 | 0.26 | 130.54 | 1.33 |
| $UF_6$ | 167.43 | 162.33 | 3.05 | 151.46 | 9.54 |
| $UI_3$ | 112.02 | 110.18 | 1.65 | 103.76 | 7.37 |
| $UI_4$ | 134.43 | 132.69 | 1.30 | 129.70 | 3.52 |
| $UO_2$ | 63.57 | 63.14 | 0.68 | 59.41 | 6.54 |
| $UO_2SO_4$ | 144.88 | 143.47 | 0.97 | 148.95 | 2.81 |
| $UOBr_2$ | 97.88 | 96.44 | 1.47 | 94.56 | 3.40 |

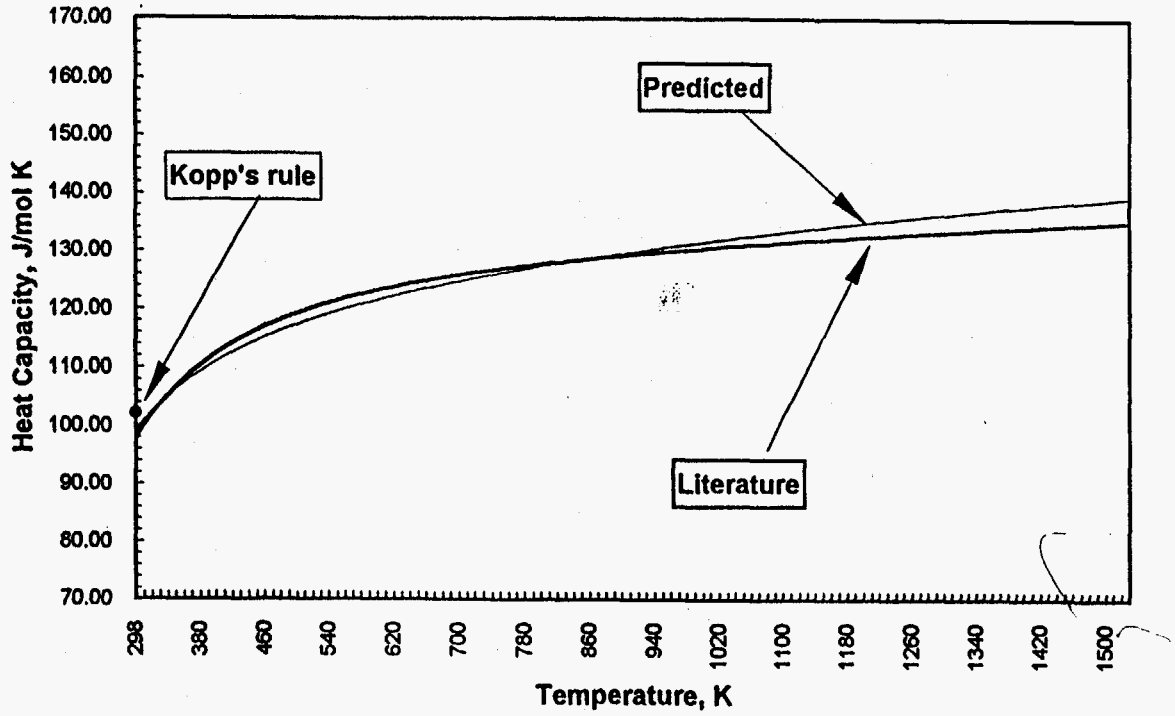


Figure 1. Heat capacity ($C_p$, *J/mol °K*) vs. temperature (*°K*) of $CaTiO_3$ for literature (From Robie et. al., 1979) and predicted values

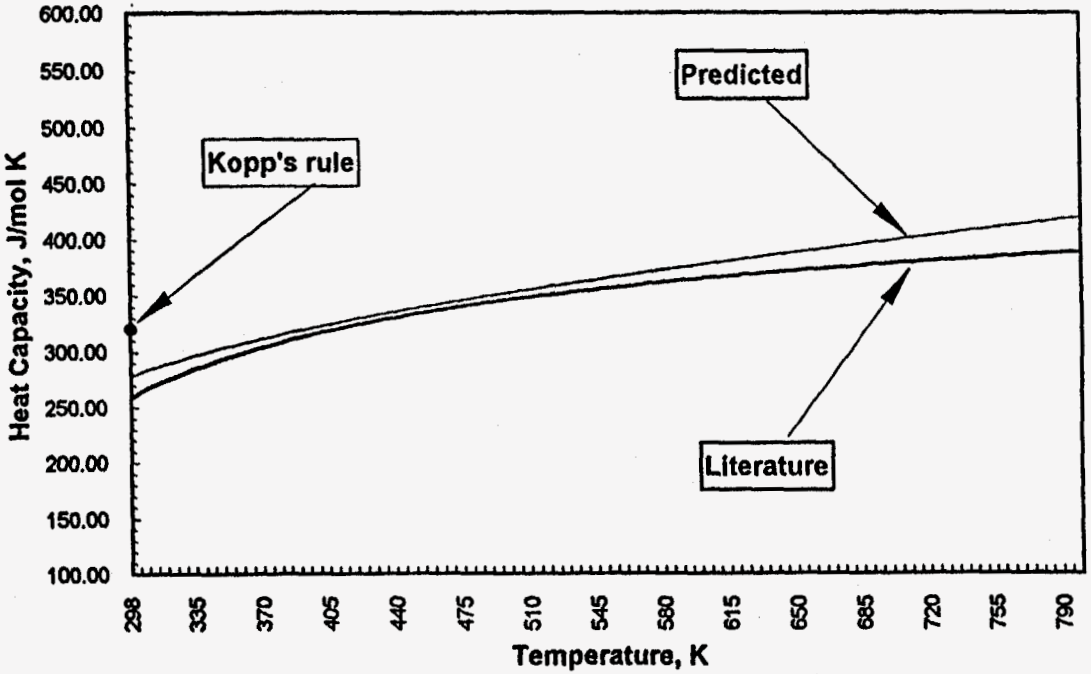


Figure 2. Heat capacity ($C_p$, *J/mol °K*) vs. temperature (*°K*) of $Fe_2(SO_4)_3$ for literature (From Robie et. al., 1979) and predicted values.

Figure 3. Heat capacity ($C_p$, *J/mol °K*) vs. temperature (*°K*) of $FeTiO_3$ for literature (From Robie et. al., 1979) and predicted values.

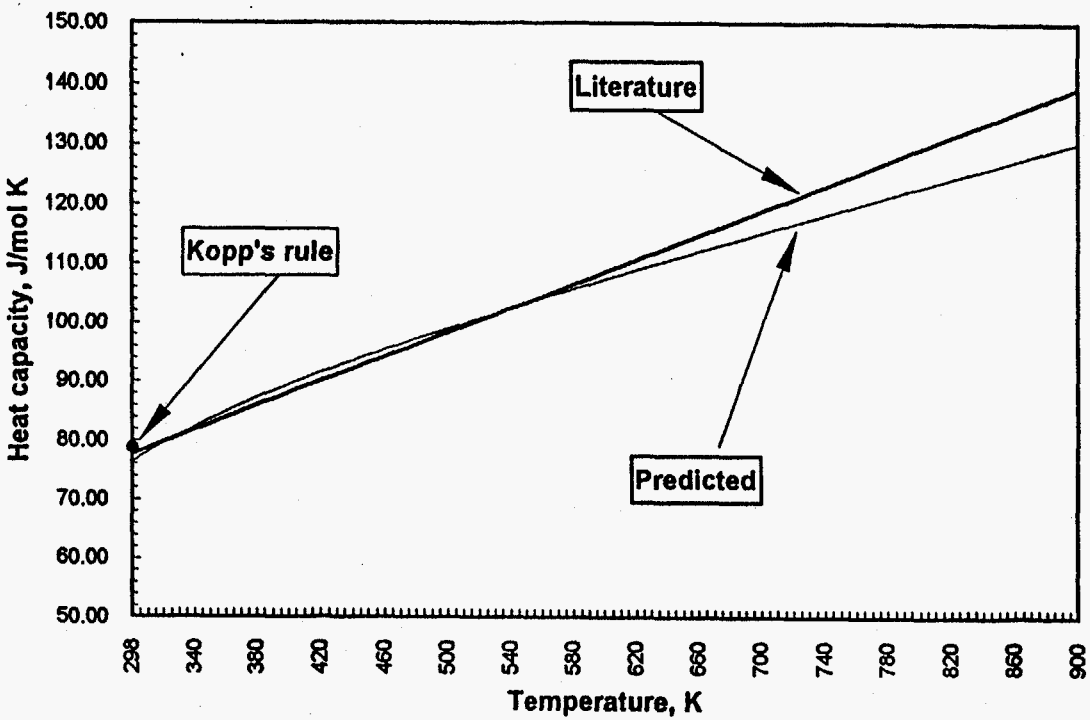


Figure 4. Heat capacity ($C_p$, *J/mol °K*) vs. temperature (*°K*) of $Mg(OH)_2$ for literature (From Robie et. al., 1979) and predicted values.

## SUPPLEMENTARY MATERIAL.

List of all the solid inorganic salts used in the regression, corresponding experimental values from the literature, prediction by the proposed method, percent error for the proposed method, prediction by Kopp's rule, and percent error for Kopp's rule for heat capacity at 298 $^{o}K$.

| COMPOUNDS | $C_{p,Literature}^{298}$ | $C_{p,predicted}^{298}$ | % Error | $C_{p,Kopp's\ rule}^{298}$ | % Error |
|---|---|---|---|---|---|
| $Ag_2CO_3$ | 111.60 | 109.98 | 1.45 | 109.62 | 1.77 |
| $Ag_2O$ | 66.31 | 70.26 | 5.96 | 68.62 | 3.49 |
| $Ag_2SO_4$ | 131.44 | 127.08 | 3.31 | 141.42 | 7.59 |
| $AgNO_2$ | 81.34 | 85.97 | 5.70 | 85.35 | 4.94 |
| $AgNO_3$ | 93.01 | 92.41 | 0.64 | 102.09 | 9.76 |
| $Al(OH)_3$ | 93.05 | 98.19 | 5.53 | 105.02 | 12.87 |
| $Al_2(SO_4)_3$ | 260.15 | 248.00 | 4.67 | 320.49 | 23.20 |
| $Al_2O_3$ | 78.81 | 77.53 | 1.61 | 102.09 | 29.55 |
| $Al_2O_3.3H_2O$ | 183.44 | 188.53 | 2.77 | 210.04 | 14.50 |
| $AlCl_3$ | 91.12 | 85.10 | 6.61 | 103.76 | 13.87 |
| $AlF_3$ | 75.45 | 76.61 | 1.54 | 88.70 | 17.57 |
| $AlI_3$ | 98.89 | 90.93 | 8.05 | 103.76 | 4.93 |
| AlOCl | 56.83 | 54.21 | 4.61 | 68.62 | 20.74 |
| $AlPO_4$ | 92.98 | 88.67 | 4.63 | 115.48 | 24.19 |
| $As_2O_3$ | 96.95 | 95.88 | 1.10 | 102.09 | 5.30 |
| $As_2O_5$ | 116.54 | 123.93 | 6.34 | 135.56 | 16.32 |
| $As_4O_6$ | 191.23 | 191.77 | 0.28 | 204.18 | 6.77 |
| $Ba(NO_3)_2$ | 151.32 | 160.79 | 6.25 | 178.24 | 17.79 |
| $Ba_2TiO_4$ | 149.13 | 150.56 | 0.95 | 144.77 | 2.93 |
| $Ba_3Al_2O_6$ | 215.35 | 216.20 | 0.39 | 230.12 | 6.86 |
| $BaBr_2$ | 76.91 | 79.52 | 3.39 | 77.82 | 1.18 |
| $BaCl_2$ | 75.17 | 77.11 | 2.59 | 77.82 | 3.53 |
| $BaCO_3$ | 87.97 | 85.94 | 2.31 | 83.68 | 4.88 |
| $BaF_2$ | 72.34 | 71.45 | 1.24 | 67.78 | 6.31 |
| $BaHfO_3$ | 108.25 | 105.86 | 2.21 | 102.09 | 5.69 |
| $BaI_2$ | 77.43 | 80.99 | 4.60 | 77.82 | 0.50 |
| BaO | 46.80 | 46.22 | 1.23 | 42.68 | 8.80 |
| $BaO.Al_2O_3$ | 113.63 | 123.76 | 8.91 | 144.77 | 27.40 |
| $BaO.SiO_2$ | 88.99 | 90.40 | 1.59 | 92.05 | 3.44 |
| $BaO.TiO_2$ | 102.38 | 104.34 | 1.91 | 102.09 | 0.29 |
| $BaO.UO_3$ | 146.81 | 132.87 | 9.50 | 118.83 | 19.06 |

| COMPOUNDS | $C_{p,Literature}^{298}$ | $C_{p,predicted}^{298}$ | % Error | $C_{p,Kopp's\ rule}^{298}$ | % Error |
|---|---|---|---|---|---|
| $BaO.V_2O_5$ | 172.78 | 173.51 | 0.42 | 178.24 | 3.16 |
| $BaO_2$ | 70.69 | 69.19 | 2.12 | 59.41 | 15.96 |
| $BaSO_4$ | 101.67 | 103.04 | 1.35 | 115.48 | 13.58 |
| $BaZrO_3$ | 105.39 | 102.27 | 2.95 | 102.09 | 3.13 |
| $2BaO.SiO_2$ | 134.06 | 134.87 | 0.60 | 150.62 | 12.36 |
| $Be(OH)_2$ | 65.55 | 64.63 | 1.40 | 78.66 | 20.01 |
| $Be_2SiO_4$ | 93.37 | 94.21 | 0.90 | 134.72 | 44.30 |
| $BeAl_2O_4$ | 104.88 | 102.55 | 2.22 | 144.77 | 38.03 |
| $BeAl_6O_{10}$ | 261.81 | 257.61 | 1.60 | 348.95 | 33.28 |
| $BeBr_2$ | 65.05 | 58.31 | 10.36 | 77.82 | 19.64 |
| $BeCl_2$ | 62.43 | 55.90 | 10.45 | 77.82 | 24.65 |
| $BeF_2$ | 51.83 | 50.24 | 3.07 | 67.78 | 30.77 |
| $BeSO_4$ | 85.60 | 81.84 | 4.40 | 115.48 | 34.90 |
| $BeSO_4.2H_2O$ | 152.82 | 155.84 | 1.97 | 187.44 | 22.65 |
| $BeSO_4.4H_2O$ | 216.42 | 229.84 | 6.20 | 259.41 | 19.86 |
| $3BeO.B_2O_3$ | 138.36 | 152.57 | 10.28 | 230.12 | 66.32 |
| $Bi_2(SO_4)_3$ | 278.82 | 278.93 | 0.04 | 320.49 | 14.95 |
| $Bi_2O_3$ | 113.46 | 108.46 | 4.40 | 102.09 | 10.02 |
| $BiBr_3$ | 100.82 | 104.17 | 3.33 | 103.76 | 2.92 |
| $BiCl_3$ | 100.42 | 100.57 | 0.14 | 103.76 | 3.33 |
| $BiF_3$ | 85.81 | 92.07 | 7.30 | 88.70 | 3.37 |
| $BiI_3$ | 105.88 | 106.39 | 0.48 | 103.76 | 1.99 |
| BiOCl | 70.16 | 69.67 | 0.70 | 68.62 | 2.20 |
| $Ca(NO_3)_2$ | 149.29 | 155.57 | 4.20 | 178.24 | 19.39 |
| $Ca(NO_3)_2.2H_2O$ | 231.58 | 229.57 | 0.87 | 250.20 | 8.04 |
| $Ca(NO_3)_2.3H_2O$ | 267.14 | 266.57 | 0.21 | 286.19 | 7.13 |
| $Ca(NO_3)_2.4H_2O$ | 300.62 | 303.57 | 0.98 | 322.17 | 7.17 |
| $Ca(OH)_2$ | 87.56 | 80.62 | 7.92 | 78.66 | 10.16 |
| $CaBr_2$ | 73.89 | 74.30 | 0.55 | 77.82 | 5.32 |
| $CaCl_2$ | 72.62 | 71.89 | 1.01 | 77.82 | 7.16 |
| $CaCO_3.MgCO_3$ | 155.18 | 156.98 | 1.16 | 167.36 | 7.85 |
| $CaF_2$ | 67.16 | 66.23 | 1.38 | 67.78 | 0.93 |
| $CaI_2$ | 77.16 | 75.78 | 1.80 | 77.82 | 0.86 |
| $CaO.2Al_2O_3$ | 193.83 | 196.07 | 1.16 | 246.86 | 27.36 |
| $CaO.2B_2O_3$ | 157.74 | 158.25 | 0.33 | 188.28 | 19.36 |
| $CaO.Al_2O_3$ | 120.55 | 118.54 | 1.67 | 144.77 | 20.08 |
| $CaO.Al_2O_3.SiO_2$ | 156.52 | 162.72 | 3.96 | 194.14 | 24.03 |
| $CaO.B_2O_3$ | 103.83 | 99.63 | 4.05 | 115.48 | 11.22 |

| COMPOUNDS | $C_{p,Literature}^{298}$ | $C_{p,predicted}^{298}$ | % Error | $C_{p,Kopp's\ rule}^{298}$ | % Error |
|---|---|---|---|---|---|
| $CaO.Cr_2O_3$ | 146.59 | 144.77 | 1.24 | 144.77 | 1.24 |
| $CaO.HfO_2$ | 105.71 | 100.64 | 4.80 | 102.09 | 3.42 |
| CaO.MgO | 79.61 | 77.54 | 2.60 | 85.35 | 7.22 |
| $CaO.MgO.2SiO_2$ | 156.05 | 165.90 | 6.31 | 184.10 | 17.97 |
| $CaO.MgO.SiO_2$ | 123.22 | 121.72 | 1.22 | 134.72 | 9.34 |
| $CaO.MoO_3$ | 117.06 | 115.82 | 1.06 | 118.83 | 1.51 |
| $CaO.TiO_2$ | 97.66 | 99.12 | 1.50 | 102.09 | 4.54 |
| $CaO.TiO_2.SiO_2$ | 138.89 | 143.30 | 3.18 | 151.46 | 9.05 |
| $CaO.UO_3$ | 130.44 | 127.65 | 2.13 | 118.83 | 8.90 |
| $CaO.V_2O_5$ | 170.74 | 168.29 | 1.44 | 178.24 | 4.39 |
| $CaSO_4.2H_2O$ | 185.99 | 171.83 | 7.62 | 187.44 | 0.78 |
| $CaSO_4.3H_2O$ | 205.10 | 208.83 | 1.82 | 223.43 | 8.94 |
| $2CaO.Al_2O_3.SiO_2$ | 195.74 | 203.72 | 4.08 | 236.81 | 20.99 |
| $2CaO.B_2O_3$ | 147.05 | 140.63 | 4.37 | 158.16 | 7.55 |
| $2CaO.Fe_2O_3$ | 194.05 | 188.88 | 2.66 | 187.44 | 3.40 |
| $2CaO.MgO.2SiO_2$ | 211.99 | 206.90 | 2.40 | 226.77 | 6.98 |
| $2CaO.P_2O_5$ | 187.70 | 186.21 | 0.79 | 214.22 | 14.13 |
| $2CaO.V_2O_5$ | 213.88 | 209.29 | 2.15 | 220.92 | 3.29 |
| $3CaO.2TiO_2$ | 239.57 | 239.24 | 0.14 | 246.86 | 3.04 |
| $3CaO.Al_2O_3$ | 209.65 | 200.54 | 4.34 | 230.12 | 9.76 |
| $3CaO.Al_2O_3.3SiO_2$ | 323.01 | 333.09 | 3.12 | 378.23 | 17.10 |
| $3CaO.B_2O_3$ | 187.77 | 181.63 | 3.27 | 200.83 | 6.96 |
| $3CaO.P_2O_5$ | 236.03 | 227.22 | 3.73 | 256.90 | 8.84 |
| $3CaO.V_2O_5$ | 257.02 | 250.29 | 2.62 | 263.59 | 2.56 |
| $3CaO.WO_3$ | 202.24 | 200.25 | 0.99 | 204.18 | 0.96 |
| $4CaO.3TiO_2$ | 337.70 | 338.36 | 0.20 | 348.95 | 3.33 |
| $Cd(NO_3)_2$ | 179.91 | 159.30 | 11.45 | 178.24 | 0.93 |
| $CdBr_2$ | 76.67 | 78.04 | 1.78 | 77.82 | 1.50 |
| $CdCl_2$ | 74.59 | 75.63 | 1.39 | 77.82 | 4.33 |
| $CdCO_3$ | 82.38 | 84.46 | 2.53 | 83.68 | 1.58 |
| $CdF_2$ | 66.90 | 69.97 | 4.59 | 67.78 | 1.32 |
| $CdI_2$ | 79.94 | 79.51 | 0.54 | 77.82 | 2.65 |
| CdO | 44.17 | 44.74 | 1.30 | 42.68 | 3.37 |
| $CdO.Al_2O_3$ | 129.87 | 122.27 | 5.85 | 144.77 | 11.47 |
| $CdO.Ga_2O_3$ | 138.47 | 140.33 | 1.34 | 144.77 | 4.54 |
| $CdO.SiO_2$ | 88.75 | 88.92 | 0.19 | 92.05 | 3.71 |
| $CdO.TiO_2$ | 98.48 | 102.85 | 4.44 | 102.09 | 3.66 |
| $CdSeO_3$ | 94.66 | 100.96 | 6.66 | 102.09 | 7.85 |

| COMPOUNDS | $C_{p,literature}^{298}$ | $C_{p,predicted}^{298}$ | % Error | $C_{p,Kopp's\ rule}^{298}$ | % Error |
|---|---|---|---|---|---|
| $CdSeO_4$ | 99.81 | 110.12 | 10.34 | 118.83 | 19.06 |
| $CdWO_4$ | 124.49 | 121.98 | 2.01 | 118.83 | 4.55 |
| $Ce_2(SO_4)_3$ | 280.75 | 279.16 | 0.57 | 320.49 | 14.15 |
| $Ce_2O_3$ | 116.99 | 108.70 | 7.09 | 102.09 | 12.74 |
| $Ce_2O_3.Al_2O_3$ | 189.57 | 186.23 | 1.76 | 204.18 | 7.71 |
| $CeBr_3$ | 100.83 | 104.29 | 3.43 | 103.76 | 2.91 |
| $CeF_3$ | 93.14 | 92.19 | 1.02 | 88.70 | 4.76 |
| $CeI_3$ | 100.43 | 106.51 | 6.05 | 103.76 | 3.32 |
| $CeO_2$ | 61.53 | 61.53 | 0.00 | 59.41 | 3.44 |
| $Co(NO_3)_2$ | 156.74 | 162.49 | 3.67 | 178.24 | 13.72 |
| $Co(OH)_2$ | 97.05 | 87.54 | 9.80 | 78.66 | 18.95 |
| $CoBr_2$ | 79.62 | 79.62 | 0.00 | 103.76 | 30.32 |
| $CoCl_2$ | 78.50 | 78.82 | 0.41 | 77.82 | 0.86 |
| $CoCO_3$ | 79.61 | 87.65 | 10.10 | 83.68 | 5.12 |
| $CoF_2$ | 68.78 | 73.16 | 6.36 | 67.78 | 1.45 |
| $CoF_3$ | 91.82 | 91.82 | 0.00 | 88.70 | 3.40 |
| $CoFe_2O_4$ | 152.54 | 154.80 | 1.48 | 144.77 | 5.09 |
| $CoO.Al_2O_3$ | 132.23 | 125.46 | 5.12 | 144.77 | 9.48 |
| $CoO.Cr_2O_3$ | 157.17 | 151.70 | 3.48 | 144.77 | 7.89 |
| $CoO.TiO_2$ | 107.78 | 106.04 | 1.61 | 102.09 | 5.28 |
| $CoSeO_3$ | 97.74 | 104.15 | 6.56 | 102.09 | 4.45 |
| $CoSO_4$ | 103.07 | 104.75 | 1.63 | 115.48 | 12.04 |
| $CoWO_4$ | 129.93 | 125.17 | 3.66 | 118.83 | 8.55. |
| $2CoO.SiO_2$ | 133.90 | 140.04 | 4.58 | 134.72 | 0.61 |
| $2CoO.TiO_2$ | 160.41 | 153.97 | 4.01 | 144.77 | 9.75 |
| $Cr(CO)_6$ | 240.13 | 239.84 | 0.12 | 171.54 | 28.56 |
| $Cr_2(SO_4)_3$ | 280.64 | 274.24 | 2.28 | 320.49 | 14.20 |
| $Cr_2O_3$ | 114.26 | 103.77 | 9.18 | 102.09 | 10.65 |
| $CrBr_2$ | 72.51 | 72.27 | 0.33 | 77.82 | 7.33 |
| $CrCl_2$ | 69.27 | 69.86 | 0.86 | 77.82 | 12.35 |
| $CrCl_3$ | 91.73 | 98.22 | 7.07 | 103.76 | 13.12 |
| $CrF_2$ | 64.63 | 64.20 | 0.67 | 67.78 | 4.87 |
| $CrI_2$ | 73.67 | 73.75 | 0.10 | 77.82 | 5.63 |
| $CrI_3$ | 111.67 | 104.04 | 6.83 | 103.76 | 7.08 |
| $CrO_3$ | 79.07 | 73.41 | 7.16 | 76.15 | 3.70 |
| $Cs_2B_2O_4$ | 138.91 | 136.81 | 1.52 | 141.42 | 1.81 |
| $Cs_2Si_2O_5$ | 176.71 | 166.54 | 5.75 | 167.36 | 5.29 |
| $Cs_2SiO_3$ | 122.22 | 122.36 | 0.11 | 117.99 | 3.47 |

| COMPOUNDS | $C_{p,Literature}^{298}$ | $C_{p,predicted}^{298}$ | % Error | $C_{p,Kopp's\ rule}^{298}$ | % Error |
|---|---|---|---|---|---|
| $Cs_2UO_4$ | 152.70 | 164.83 | 7.95 | 144.77 | 5.19 |
| $Cu_2O$ | 63.54 | 59.93 | 5.68 | 68.62 | 7.99 |
| $Cu_2O.Al_2O_3$ | 142.15 | 137.47 | 3.29 | 170.71 | 20.09 |
| $Cu_2O.Ga_2O_3$ | 139.97 | 155.52 | 11.11 | 170.71 | 21.96 |
| $CuBr_2$ | 75.77 | 76.21 | 0.59 | 77.82 | 2.71 |
| $CuCl_2$ | 71.74 | 73.81 | 2.89 | 77.82 | 8.48 |
| $CuF_2$ | 65.12 | 66.68 | 2.39 | 67.78 | 4.08 |
| $CuFe_2O_4$ | 148.75 | 149.79 | 0.70 | 144.77 | 2.68 |
| CuI | 54.18 | 48.82 | 9.89 | 51.88 | 4.24 |
| CuO | 42.26 | 42.92 | 1.57 | 42.68 | 1.00 |
| $CuO.Al_2O_3$ | 127.64 | 120.45 | 5.63 | 144.77 | 13.42 |
| $CuO.Cr_2O_3$ | 148.00 | 146.69 | 0.88 | 144.77 | 2.18 |
| $CuO.CuSO_4$ | 140.09 | 142.66 | 1.83 | 158.16 | 12.90 |
| $CuO.Ga_2O_3$ | 134.98 | 138.51 | 2.61 | 144.77 | 7.25 |
| $CuSO_4$ | 98.77 | 99.74 | 0.98 | 115.48 | 16.92 |
| $Dy_2O_3$ | 116.21 | 113.14 | 2.64 | 102.09 | 12.15 |
| $DyCl_3$ | 97.03 | 102.91 | 6.06 | 103.76 | 6.94 |
| $DyF_3$ | 94.15 | 94.41 | 0.28 | 88.70 | 5.79 |
| $ErCl_3$ | 103.29 | 110.36 | 6.85 | 103.76 | 0.46 |
| $ErF_3$ | 111.53 | 101.87 | 8.67 | 88.70 | 20.47 |
| $Eu_2O_3$ | 124.65 | 128.41 | 3.02 | 102.09 | 18.10 |
| $EuBr_2$ | 82.39 | 82.21 | 0.21 | 77.82 | 5.54 |
| $EuBr_3$ | 110.66 | 114.15 | 3.15 | 103.76 | 6.24 |
| $EuCl_3$ | 106.92 | 110.54 | 3.39 | 103.76 | 2.95 |
| $EuCl_3.6H_2O$ | 366.91 | 332.54 | 9.37 | 319.66 | 12.88 |
| $EuF_3$ | 99.49 | 102.05 | 2.57 | 88.70 | 10.84 |
| EuO | 48.74 | 48.92 | 0.36 | 42.68 | 12.45 |
| $Fe(OH)_2$ | 86.23 | 82.56 | 4.26 | 78.66 | 8.78 |
| $Fe_2(SO_4)_3$ | 257.80 | 277.34 | 7.58 | 320.49 | 24.32 |
| $Fe_2O_3$ | 104.69 | 106.87 | 2.08 | 102.09 | 2.49 |
| $Fe_2SiO_4$ | 132.90 | 130.06 | 2.14 | 134.72 | 1.37 |
| $Fe_3O_4$ | 151.75 | 149.81 | 1.27 | 144.77 | 4.60 |
| $FeAl_2O_4$ | 123.46 | 120.47 | 2.42 | 144.77 | 17.25 |
| $FeBr_2$ | 80.23 | 76.24 | 4.98 | 77.82 | 3.00 |
| $FeCl_2$ | 76.50 | 73.83 | 3.48 | 77.82 | 1.73 |
| $FeCl_3$ | 96.90 | 99.77 | 2.96 | 103.76 | 7.08 |
| $FeCO_3$ | 82.06 | 82.66 | 0.73 | 83.68 | 1.97 |
| $FeCr_2O_4$ | 133.75 | 146.71 | 9.69 | 144.77 | 8.24 |

| COMPOUNDS | $C_{p,Literature}^{298}$ | $C_{p,predicted}^{298}$ | % Error | $C_{p,Kopp's\ rule}^{298}$ | % Error |
|---|---|---|---|---|---|
| $FeF_2$ | 68.17 | 68.17 | 0.01 | 67.78 | 0.58 |
| $FeF_3$ | 91.64 | 91.28 | 0.40 | 88.70 | 3.21 |
| $FeMoO_4$ | 117.59 | 117.76 | 0.14 | 118.83 | 1.05 |
| FeO | 48.02 | 42.94 | 10.58 | 42.68 | 11.12 |
| FeO(OH) | 74.31 | 73.24 | 1.43 | 69.04 | 7.09 |
| FeOCl | 77.03 | 68.88 | 10.58 | 68.62 | 10.92 |
| $FeSO_4$ | 100.29 | 99.76 | 0.52 | 115.48 | 15.15 |
| $FeTiO_3$ | 99.52 | 106.41 | 6.92 | 102.09 | 2.58 |
| $FeWO_4$ | 114.26 | 120.18 | 5.18 | 118.83 | 4.00 |
| $Ga_2O_3$ | 93.83 | 95.59 | 1.87 | 102.09 | 8.80 |
| $GaBr_3$ | 101.65 | 97.74 | 3.84 | 103.76 | 2.08 |
| $Gd_2O_3$ | 105.50 | 101.85 | 3.46 | 102.09 | 3.23 |
| $GdBr_3$ | 96.91 | 100.87 | 4.09 | 103.76 | 7.07 |
| $GdCl_3$ | 97.75 | 97.26 | 0.50 | 103.76 | 6.15 |
| $GdF_3$ | 88.38 | 88.77 | 0.43 | 88.70 | 0.36 |
| $GdI_3$ | 98.66 | 103.08 | 4.49 | 103.76 | 5.17 |
| GdOCl | 68.34 | 66.37 | 2.87 | 68.62 | 0.41 |
| $GeI_2$ | 81.62 | 80.36 | 1.55 | 77.82 | 4.66 |
| $GeI_4$ | 126.05 | 123.76 | 1.82 | 129.70 | 2.89 |
| GeO | 44.32 | 45.59 | 2.85 | 42.68 | 3.71 |
| $GeO_2$ | 51.93 | 54.22 | 4.41 | 59.41 | 14.42 |
| $H_2WO_4$ | 104.08 | 110.07 | 5.76 | 112.13 | 7.74 |
| $H_3BO_3$ | 81.19 | 78.56 | 3.25 | 90.37 | 11.31 |
| $H_3PO_4$ | 106.23 | 99.15 | 6.66 | 118.41 | 11.47 |
| $HfBr_4$ | 127.60 | 126.23 | 1.08 | 129.70 | 1.65 |
| $HfCl_4$ | 120.53 | 121.42 | 0.74 | 129.70 | 7.61 |
| $HfF_4$ | 100.43 | 110.09 | 9.62 | 109.62 | 9.16 |
| $HfI_2$ | 61.89 | 61.89 | 0.00 | 77.82 | 25.73 |
| $HfI_4$ | 144.32 | 129.18 | 10.49 | 129.70 | 10.13 |
| $HfO_2$ | 60.28 | 59.63 | 1.07 | 59.41 | 1.44 |
| $Hg_2Br_2$ | 104.65 | 105.33 | 0.65 | 103.76 | 0.85 |
| $Hg_2Cl_2$ | 101.54 | 102.92 | 1.36 | 103.76 | 2.19 |
| $Hg_2F_2$ | 100.31 | 97.26 | 3.05 | 93.72 | 6.57 |
| $Hg_2I_2$ | 105.81 | 106.81 | 0.94 | 103.76 | 1.93 |
| $HgBr_2$ | 75.35 | 77.17 | 2.42 | 77.82 | 3.28 |
| $HgCl_2$ | 73.91 | 74.77 | 1.16 | 77.82 | 5.30 |
| $HgI_2$ | 77.75 | 78.65 | 1.16 | 77.82 | 0.10 |
| HgO | 43.91 | 43.88 | 0.07 | 42.68 | 2.81 |

| COMPOUNDS | $C_{p,Literature}^{298}$ | $C_{p,predicted}^{298}$ | % Error | $C_{p,Kopp's\ rule}^{298}$ | % Error |
|---|---|---|---|---|---|
| $HgSeO_3$ | 102.13 | 100.10 | 1.99 | 102.09 | 0.04 |
| $HgSO_4$ | 102.22 | 100.70 | 1.49 | 115.48 | 12.97 |
| $Ho_2O_3$ | 114.96 | 113.44 | 1.32 | 102.09 | 11.20 |
| $HoBr_3$ | 98.79 | 106.67 | 7.98 | 103.76 | 5.04 |
| $HoCl_3$ | 96.18 | 103.06 | 7.15 | 103.76 | 7.88 |
| $HoCl_3.6H_2O$ | 347.30 | 325.06 | 6.40 | 319.66 | 7.96 |
| $HoF_3$ | 91.22 | 94.56 | 3.67 | 88.70 | 2.76 |
| $In_2O_3$ | 100.33 | 100.58 | 0.25 | 102.09 | 1.75 |
| InBr | 50.99 | 50.31 | 1.33 | 51.88 | 1.75 |
| $InBr_3$ | 98.22 | 100.23 | 2.05 | 103.76 | 5.65 |
| InCl | 47.62 | 49.11 | 3.13 | 51.88 | 8.95 |
| $InCl_2$ | 73.54 | 73.54 | 0.00 | 77.82 | 5.82 |
| $InCl_3$ | 95.24 | 96.63 | 1.45 | 103.76 | 8.94 |
| $InF_3$ | 92.02 | 88.13 | 4.23 | 88.70 | 3.60 |
| InI | 51.86 | 51.05 | 1.56 | 51.88 | 0.04 |
| $IrBr_3$ | 105.44 | 97.44 | 7.59 | 103.76 | 1.59 |
| $IrCl_3$ | 85.82 | 93.83 | 9.33 | 103.76 | 20.91 |
| $IrO_2$ | 55.58 | 55.58 | 0.00 | 59.41 | 6.90 |
| $K_2B_2O_4$ | 141.88 | 136.68 | 3.67 | 141.42 | 0.33 |
| $K_2B_6O_{10}$ | 265.30 | 253.93 | 4.29 | 287.02 | 8.19 |
| $K_2B_8O1_3$ | 318.93 | 312.55 | 2.00 | 359.82 | 12.82 |
| $K_2CO_3$ | 114.25 | 117.77 | 3.08 | 109.62 | 4.05 |
| $K_2CrO_4$ | 146.04 | 151.46 | 3.72 | 144.77 | 0.87 |
| $K_2HPO_4$ | 143.47 | 144.37 | 0.63 | 151.04 | 5.28 |
| $K_2O.Al_2O_3.2SiO_2$ | 239.72 | 243.95 | 1.76 | 269.45 | 12.40 |
| $K_2O.Al_2O_3.4SiO_2$ | 328.45 | 332.31 | 1.18 | 368.19 | 12.10 |
| $K_2O.Fe_2O_3$ | 187.85 | 184.93 | 1.56 | 170.71 | 9.13 |
| $K_2Si_2O_5$ | 160.85 | 166.42 | 3.46 | 167.36 | 4.05 |
| $K_2SiO_3$ | 118.62 | 122.23 | 3.04 | 117.99 | 0.53 |
| $K_2SO_4$ | 131.57 | 134.87 | 2.52 | 141.42 | 7.49 |
| $K_2WO_4$ | 150.79 | 155.29 | 2.98 | 144.77 | 4.00 |
| $K_3AlCl_6$ | 249.02 | 248.52 | 0.20 | 259.41 | 4.17 |
| $K_3AlF_6$ | 221.66 | 231.53 | 4.45 | 229.28 | 3.44 |
| $K_3PO_4$ | 164.60 | 166.99 | 1.45 | 167.36 | 1.68 |
| $KAl(SO_4)_2$ | 192.91 | 191.44 | 0.77 | 230.96 | 19.72 |
| $KAlCl_4$ | 156.48 | 139.57 | 10.80 | 155.64 | 0.53 |
| $KBF_4$ | 114.70 | 118.79 | 3.57 | 120.92 | 5.42 |
| KCl | 51.58 | 54.47 | 5.60 | 51.88 | 0.58 |

| COMPOUNDS | $C_{p,Literature}^{298}$ | $C_{p,predicted}^{298}$ | % Error | $C_{p,Kopp's\ rule}^{298}$ | % Error |
|---|---|---|---|---|---|
| $KClO_3$ | 100.45 | 102.68 | 2.22 | 102.09 | 1.63 |
| $KClO_4$ | 112.37 | 115.11 | 2.44 | 118.83 | 5.74 |
| $KH_2PO_4$ | 116.49 | 121.76 | 4.53 | 134.72 | 15.65 |
| $KHCO_3$ | 90.05 | 91.04 | 1.11 | 93.30 | 3.62 |
| $KHF_2$ | 76.89 | 80.67 | 4.91 | 77.40 | 0.66 |
| KI | 52.96 | 56.41 | 6.51 | 51.88 | 2.04 |
| $KNO_3$ | 95.87 | 96.31 | 0.46 | 102.09 | 6.49 |
| $KO_2$ | 78.23 | 73.48 | 6.07 | 59.41 | 24.05 |
| KOH | 64.93 | 58.83 | 9.39 | 52.30 | 19.45 |
| $La_2O_3$ | 108.77 | 104.68 | 3.76 | 102.09 | 6.14 |
| $LaBr_3$ | 99.59 | 102.29 | 2.70 | 103.76 | 4.19 |
| $LaCl_3$ | 98.13 | 98.68 | 0.56 | 103.76 | 5.74 |
| $LaF_3$ | 90.36 | 90.18 | 0.20 | 88.70 | 1.84 |
| $LaI_3$ | 99.10 | 104.50 | 5.45 | 103.76 | 4.71 |
| LaOCl | 68.97 | 67.79 | 1.72 | 68.62 | 0.52 |
| $LaPO_4$ | 101.64 | 102.25 | 0.60 | 115.48 | 13.62 |
| $Li_2B_2O_4$ | 120.82 | 126.87 | 5.01 | 118.83 | 1.65 |
| $Li_2B_4O_7$ | 170.34 | 175.21 | 2.86 | 214.22 | 25.76 |
| $Li_2B_6O_{10}$ | 291.00 | 264.69 | 9.04 | 219.24 | 24.66 |
| $Li_2B_8O13_3$ | 320.65 | 333.60 | 4.04 | 269.45 | 15.97 |
| $Li_2BeF_4$ | 134.97 | 133.42 | 1.15 | 161.50 | 19.66 |
| $Li_2CO_3$ | 97.96 | 97.68 | 0.30 | 109.62 | 11.90 |
| $Li_2HfO_3$ | 111.87 | 117.59 | 5.11 | 128.03 | 14.44 |
| $Li_2Nb_2O_6$ | 198.55 | 204.22 | 2.86 | 204.18 | 2.83 |
| $Li_2O$ | 54.07 | 57.96 | 7.18 | 68.62 | 26.90 |
| $Li_2O.Al_2O_3.2SiO_2$ | 226.50 | 220.33 | 2.72 | 301.25 | 33.00 |
| $Li_2O.Al_2O_3.4SiO_2$ | 317.69 | 305.18 | 3.94 | 431.79 | 35.91 |
| $Li_2Si_2O_5$ | 138.62 | 146.32 | 5.55 | 167.36 | 20.73 |
| $Li_2SiO_3$ | 99.90 | 102.14 | 2.24 | 117.99 | 18.11 |
| $Li_2SO_4$ | 117.14 | 114.78 | 2.01 | 141.42 | 20.73 |
| $Li_2Ta_2O_6$ | 200.14 | 197.02 | 1.56 | 204.18 | 2.02 |
| $Li_2TiO_3$ | 108.48 | 116.07 | 7.00 | 128.03 | 18.02 |
| $Li_2WO_4$ | 133.34 | 135.20 | 1.39 | 144.77 | 8.57 |
| $Li_2ZrO_3$ | 110.20 | 114.01 | 3.45 | 128.03 | 16.18 |
| $Li_3AlF_6$ | 202.30 | 201.38 | 0.45 | 229.28 | 13.34 |
| $LiBeF_3$ | 92.61 | 91.83 | 0.84 | 114.64 | 23.79 |
| LiBr | 49.06 | 45.63 | 7.00 | 51.88 | 5.75 |
| LiCl | 48.10 | 44.42 | 7.64 | 51.88 | 7.87 |

| COMPOUNDS | $C_{p,Literature}^{298}$ | $C_{p,predicted}^{298}$ | % Error | $C_{p,Kopp's\ rule}^{298}$ | % Error |
|---|---|---|---|---|---|
| $LiClO_4$ | 104.94 | 105.06 | 0.12 | 118.83 | 13.24 |
| LiF | 41.85 | 41.59 | 0.61 | 46.86 | 11.98 |
| LiI | 51.80 | 46.36 | 10.50 | 51.88 | 0.15 |
| $LiNO_3$ | 89.11 | 86.26 | 3.20 | 102.09 | 14.56 |
| LiOH | 49.75 | 48.79 | 1.93 | 52.30 | 5.13 |
| $Lu_2O_3$ | 101.72 | 101.05 | 0.65 | 102.09 | 0.36 |
| $LuF_3$ | 87.04 | 88.37 | 1.53 | 88.70 | 1.91 |
| $Mg(NO_3)_2$ | 141.90 | 151.10 | 6.48 | 178.24 | 25.61 |
| $Mg(OH)_2$ | 77.49 | 76.15 | 1.73 | 78.66 | 1.50 |
| $Mg_2SiO_4$ | 118.43 | 117.25 | 1.00 | 134.72 | 13.76 |
| $Mg_2TiO_4$ | 128.17 | 131.19 | 2.35 | 144.77 | 12.94 |
| $Mg_2V_2O_7$ | 202.26 | 200.35 | 0.94 | 220.92 | 9.23 |
| $Mg_3P_2O_8$ | 213.09 | 213.82 | 0.34 | 256.90 | 20.56 |
| $MgAl_2O_4$ | 115.94 | 114.07 | 1.61 | 144.77 | 24.87 |
| $MgBr_2$ | 74.67 | 69.83 | 6.48 | 77.82 | 4.23 |
| $MgCl_2$ | 71.29 | 67.43 | 5.41 | 77.82 | 9.17 |
| $MgCO_3$ | 75.40 | 76.26 | 1.13 | 83.68 | 10.98 |
| $MgCr_2O_4$ | 126.72 | 140.30 | 10.72 | 144.77 | 14.24 |
| $MgF_2$ | 61.33 | 61.76 | 0.70 | 67.78 | 10.51 |
| $MgFe_2O_4$ | 137.76 | 143.41 | 4.10 | 144.77 | 5.09 |
| $MgI_2$ | 74.78 | 71.31 | 4.65 | 77.82 | 4.07 |
| $MgMoO_4$ | 110.88 | 111.35 | 0.42 | 118.83 | 7.16 |
| MgO | 37.25 | 36.54 | 1.91 | 42.68 | 14.58 |
| $MgSiO_3$ | 81.85 | 80.72 | 1.39 | 92.05 | 12.45 |
| $MgSO_4$ | 95.57 | 93.36 | 2.31 | 115.48 | 20.83 |
| $MgTi_2O_5$ | 146.60 | 152.76 | 4.21 | 161.50 | 10.17 |
| $MgTiO_3$ | 91.17 | 94.65 | 3.82 | 102.09 | 11.98 |
| $MgV_2O_6$ | 159.87 | 163.82 | 2.47 | 178.24 | 11.49 |
| $MgWO_4$ | 109.83 | 113.78 | 3.59 | 118.83 | 8.19 |
| $Mn_2O_3$ | 99.02 | 99.77 | 0.76 | 102.09 | 3.10 |
| $Mn_2SiO_4$ | 129.87 | 130.45 | 0.45 | 134.72 | 3.74 |
| $Mn_2TiO_4$ | 144.52 | 144.38 | 0.09 | 144.77 | 0.17 |
| $Mn_3O_4$ | 140.48 | 142.90 | 1.73 | 144.77 | 3.05 |
| $MnAl_2O_4$ | 124.60 | 120.67 | 3.16 | 144.77 | 16.18 |
| $MnBr_2$ | 75.30 | 76.43 | 1.50 | 77.82 | 3.35 |
| $MnCl_2$ | 73.01 | 74.03 | 1.39 | 77.82 | 6.59 |
| $MnF_2$ | 62.71 | 68.36 | 9.01 | 67.78 | 8.09 |
| $MnMoO_4$ | 124.07 | 117.95 | 4.93 | 118.83 | 4.22 |

| COMPOUNDS | $C_{p,Literature}^{298}$ | $C_{p,predicted}^{298}$ | % Error | $C_{p,Kopp's\ rule}^{298}$ | % Error |
|---|---|---|---|---|---|
| $MnO.Fe_2O_3$ | 149.19 | 150.01 | 0.55 | 144.77 | 2.97 |
| $MnSiO_3$ | 86.32 | 87.32 | 1.15 | 92.05 | 6.63 |
| $MnSO_4$ | 100.37 | 99.96 | 0.41 | 115.48 | 15.06 |
| $MnTiO_3$ | 99.78 | 101.25 | 1.48 | 102.09 | 2.32 |
| $MnWO_4$ | 124.07 | 120.37 | 2.98 | 118.83 | 4.22 |
| $Mo(CO)_6$ | 241.96 | 241.24 | 0.30 | 171.54 | 29.10 |
| $MoBr_2$ | 79.69 | 79.30 | 0.49 | 77.82 | 2.35 |
| $MoBr_3$ | 105.37 | 103.84 | 1.46 | 103.76 | 1.52 |
| $MoBr_4$ | 133.02 | 131.50 | 1.15 | 129.70 | 2.49 |
| $MoCl_2$ | 74.58 | 76.89 | 3.10 | 77.82 | 4.35 |
| $MoCl_3$ | 94.87 | 100.23 | 5.65 | 103.76 | 9.38 |
| $MoCl_4$ | 124.40 | 126.68 | 1.84 | 129.70 | 4.26 |
| $MoCl_5$ | 156.13 | 159.96 | 2.45 | 155.64 | 0.31 |
| $MoF_3$ | 95.21 | 91.73 | 3.65 | 88.70 | 6.84 |
| $MoF_4$ | 125.04 | 115.36 | 7.74 | 109.62 | 12.33 |
| $MoF_5$ | 149.63 | 145.80 | 2.56 | 130.54 | 12.76 |
| $MoI_2$ | 82.70 | 80.77 | 2.32 | 77.82 | 5.89 |
| $MoI_3$ | 106.40 | 106.05 | 0.33 | 103.76 | 2.47 |
| $MoO_2Cl_2$ | 107.65 | 105.71 | 1.80 | 111.29 | 3.39 |
| $MoO_3$ | 75.12 | 74.82 | 0.41 | 76.15 | 1.37 |
| $Na_2B_2O_4$ | 131.68 | 128.50 | 2.41 | 141.42 | 7.40 |
| $Na_2B_4O_7$ | 186.85 | 187.12 | 0.15 | 214.22 | 14.65 |
| $Na_2B_6O_{10}$ | 243.61 | 245.75 | 0.88 | 287.02 | 17.82 |
| $Na_2B_8O13$ | 304.75 | 304.37 | 0.12 | 359.82 | 18.07 |
| $Na_2CO_3$ | 111.30 | 109.59 | 1.53 | 109.62 | 1.51 |
| $Na_2Cr_2O_4$ | 178.78 | 173.64 | 2.88 | 170.71 | 4.52 |
| $Na_2CrO_4$ | 142.76 | 143.29 | 0.37 | 144.77 | 1.41 |
| $Na_2Mo_2O_7$ | 216.66 | 219.50 | 1.31 | 220.92 | 1.97 |
| $Na_2MoO_4$ | 141.43 | 144.69 | 2.30 | 144.77 | 2.36 |
| $Na_2O$ | 68.54 | 69.87 | 1.94 | 68.62 | 0.11 |
| $Na_2O.Al_2O_3.4SiO_2$ | 311.72 | 324.13 | 3.98 | 368.19 | 18.12 |
| $Na_2O.Al_2O_3.6SiO_2$ | 409.54 | 412.50 | 0.72 | 466.93 | 14.02 |
| $Na_2O.UO_3$ | 146.71 | 156.52 | 6.69 | 144.77 | 1.33 |
| $Na_2O_2$ | 88.92 | 92.84 | 4.41 | 85.35 | 4.01 |
| $Na_2P_2O_6$ | 174.44 | 174.08 | 0.20 | 197.48 | 13.21 |
| $Na_2Si_2O_5$ | 156.44 | 158.24 | 1.15 | 167.36 | 6.98 |
| $Na_2SiO_3$ | 111.78 | 114.06 | 2.04 | 117.99 | 5.56 |
| $Na_2SO_3$ | 120.08 | 120.08 | 0.00 | 124.68 | 3.84 |

| COMPOUNDS | $C_{p,Literature}^{298}$ | $C_{p,predicted}^{298}$ | % Error | $C_{p,Kopp's\ rule}^{298}$ | % Error |
|---|---|---|---|---|---|
| $Na_2SO_4$ | 128.34 | 126.70 | 1.28 | 141.42 | 10.19 |
| $Na_2Ti_2O_5$ | 193.11 | 187.16 | 3.08 | 187.44 | 2.93 |
| $Na_2Ti_3O_7$ | 252.21 | 245.69 | 2.58 | 246.86 | 2.12 |
| $Na_2TiO_3$ | 131.18 | 128.62 | 1.95 | 128.03 | 2.40 |
| $Na_2V_2O_6$ | 195.10 | 198.42 | 1.70 | 204.18 | 4.65 |
| $Na_2WO_4$ | 141.75 | 147.11 | 3.78 | 144.77 | 2.13 |
| $Na_3AlF_6$ | 222.72 | 219.26 | 1.55 | 229.28 | 2.95 |
| $Na_4P_2O_7$ | 241.24 | 243.96 | 1.13 | 266.10 | 10.31 |
| $Na_4V_2O_7$ | 269.74 | 268.51 | 0.46 | 272.80 | 1.13 |
| $Na_5Al_3F_{14}$ | 461.92 | 467.57 | 1.22 | 500.41 | 8.33 |
| $Na_6As_2O_8$ | 340.94 | 333.55 | 2.17 | 341.41 | 0.14 |
| $Na_6P_2O_8$ | 306.63 | 313.83 | 2.35 | 334.72 | 9.16 |
| $Na_6V_2O_8$ | 329.62 | 338.59 | 2.72 | 341.41 | 3.58 |
| $NaBF_4$ | 119.94 | 114.70 | 4.37 | 120.92 | 0.82 |
| NaBr | 51.43 | 51.59 | 0.31 | 51.88 | 0.88 |
| $NaClO_3$ | 100.82 | 98.59 | 2.21 | 102.09 | 1.26 |
| $NaClO_4$ | 111.03 | 111.02 | 0.01 | 118.83 | 7.02 |
| NaF | 46.91 | 47.55 | 1.36 | 46.86 | 0.11 |
| $NaHCO_3$ | 87.95 | 86.95 | 1.13 | 93.30 | 6.09 |
| NaI | 49.53 | 52.32 | 5.65 | 51.88 | 4.76 |
| $NaNO_3$ | 93.00 | 92.22 | 0.84 | 102.09 | 9.77 |
| $NaO_2$ | 72.17 | 69.39 | 3.85 | 59.41 | 17.68 |
| $NbCl_3$ | 97.40 | 97.40 | 0.00 | 103.76 | 6.53 |
| $NbCl_4$ | 119.81 | 121.12 | 1.10 | 129.70 | 8.26 |
| $NbCl_5$ | 147.90 | 150.36 | 1.66 | 155.64 | 5.24 |
| $NbF_5$ | 149.66 | 136.20 | 9.00 | 130.54 | 12.78 |
| $NbO_2$ | 57.68 | 59.34 | 2.89 | 59.41 | 3.01 |
| $NbOCl_2$ | 93.21 | 90.23 | 3.19 | 94.56 | 1.45 |
| $NbOCl_3$ | 119.81 | 119.47 | 0.28 | 120.50 | 0.57 |
| $Nd_2O_3$ | 111.32 | 107.16 | 3.74 | 102.09 | 8.29 |
| $Nd_2O_3.2ZrO_2$ | 223.33 | 219.26 | 1.82 | 220.92 | 1.08 |
| $NdBr_3$ | 104.13 | 103.52 | 0.58 | 103.76 | 0.35 |
| $NdCl_3$ | 99.16 | 99.92 | 0.76 | 103.76 | 4.64 |
| $NdF_3$ | 92.43 | 91.42 | 1.09 | 88.70 | 4.03 |
| $NdI_3$ | 98.73 | 105.74 | 7.09 | 103.76 | 5.10 |
| NdOCl | 69.85 | 69.02 | 1.18 | 68.62 | 1.76 |
| $NH_4ClO_4$ | 128.07 | 140.15 | 9.43 | 157.32 | 22.83 |
| $(NH_4)_2SO_4$ | 187.21 | 184.95 | 1.21 | 218.40 | 16.66 |

| COMPOUNDS | $C_{p,Literature}^{298}$ | $C_{p,predicted}^{298}$ | % Error | $C_{p,Kopp's\ rule}^{298}$ | % Error |
|---|---|---|---|---|---|
| $Ni_2SiO_4$ | 126.95 | 131.75 | 3.78 | 134.72 | 6.13 |
| $NiAl_2O_4$ | 131.53 | 121.32 | 7.76 | 144.77 | 10.06 |
| $NiBr_2$ | 75.40 | 77.08 | 2.23 | 77.82 | 3.21 |
| $NiCl_2$ | 71.68 | 74.68 | 4.17 | 77.82 | 8.56 |
| $NiCO_3$ | 86.40 | 83.51 | 3.35 | 83.68 | 3.15 |
| $NiCr_2O_4$ | 148.77 | 147.55 | 0.82 | 144.77 | 2.69 |
| $NiFe_2O_4$ | 159.14 | 150.66 | 5.33 | 144.77 | 9.03 |
| $NiI_2$ | 77.41 | 78.56 | 1.48 | 77.82 | 0.53 |
| NiO | 44.28 | 43.78 | 1.13 | 42.68 | 3.63 |
| $NiSeO_3$ | 97.33 | 100.01 | 2.75 | 102.09 | 4.89 |
| $NiSO_4$ | 97.48 | 100.61 | 3.21 | 115.48 | 18.47 |
| $NiTiO_3$ | 99.25 | 101.90 | 2.66 | 102.09 | 2.86 |
| $NiWO_4$ | 121.60 | 121.02 | 0.47 | 118.83 | 2.28 |
| $NpCl_3$ | 101.61 | 109.32 | 7.58 | 103.76 | 2.11 |
| $NpCl_4$ | 120.86 | 123.51 | 2.19 | 129.70 | 7.32 |
| $NpF_3$ | 108.52 | 100.82 | 7.10 | 88.70 | 18.26 |
| $NpF_6$ | 167.44 | 162.09 | 3.20 | 151.46 | 9.54 |
| $NpO_2$ | 64.14 | 61.73 | 3.77 | 59.41 | 7.37 |
| $NpO_3.H_2O$ | 118.06 | 123.41 | 4.53 | 112.13 | 5.02 |
| $NpOCl_2$ | 92.85 | 92.62 | 0.25 | 94.56 | 1.84 |
| $Pb_2SiO_4$ | 136.90 | 139.14 | 1.64 | 134.72 | 1.59 |
| $Pb_4SiO_6$ | 229.70 | 234.09 | 1.91 | 220.08 | 4.19 |
| $PbB_4O_7$ | 151.71 | 164.73 | 8.58 | 188.28 | 24.10 |
| $PbBr_2$ | 79.47 | 80.77 | 1.64 | 77.82 | 2.08 |
| $PbCl_2$ | 77.14 | 78.37 | 1.59 | 77.82 | 0.88 |
| $PbF_2$ | 72.29 | 72.70 | 0.57 | 67.78 | 6.24 |
| $PbI_2$ | 77.57 | 82.25 | 6.03 | 77.82 | 0.32 |
| $PbO.PbCO_3$ | 133.23 | 134.68 | 1.09 | 126.36 | 5.16 |
| $PbO_2$ | 60.99 | 60.99 | 0.00 | 59.41 | 2.58 |
| $PbSiO_3$ | 89.10 | 91.66 | 2.88 | 92.05 | 3.31 |
| $PbSO_4$ | 102.98 | 104.30 | 1.28 | 115.48 | 12.13 |
| $PbSO_4.2PbO$ | 205.84 | 199.26 | 3.20 | 200.83 | 2.43 |
| $PbSO_4.3PbO$ | 251.55 | 246.73 | 1.91 | 243.51 | 3.19 |
| $PbSO_4.PbO$ | 160.15 | 151.78 | 5.23 | 158.16 | 1.24 |
| $PbTiO_3$ | 104.38 | 105.59 | 1.16 | 102.09 | 2.20 |
| $PbWO_4$ | 119.62 | 124.72 | 4.26 | 118.83 | 0.67 |
| $PdCl_2$ | 75.27 | 74.45 | 1.09 | 77.82 | 3.39 |
| $PdI_2$ | 75.06 | 78.33 | 4.37 | 77.82 | 3.68 |

| COMPOUNDS | $C_{p,Literature}^{298}$ | $C_{p,predicted}^{298}$ | % Error | $C_{p,Kopp's\ rule}^{298}$ | % Error |
|---|---|---|---|---|---|
| PdO | 46.02 | 43.56 | 5.34 | 42.68 | 7.26 |
| $Pr_2O_3$ | 116.61 | 107.65 | 7.69 | 102.09 | 12.46 |
| $PrBr_3$ | 101.65 | 103.77 | 2.08 | 103.76 | 2.08 |
| $PrCl_3$ | 98.92 | 100.16 | 1.25 | 103.76 | 4.90 |
| $PrF_3$ | 92.48 | 91.66 | 0.88 | 88.70 | 4.09 |
| $PrI_3$ | 99.55 | 105.98 | 6.46 | 103.76 | 4.23 |
| $PrO_2$ | 72.92 | 72.92 | 0.00 | 59.41 | 18.52 |
| $PtBr_2$ | 75.90 | 76.85 | 1.26 | 77.82 | 2.54 |
| $PtBr_3$ | 100.36 | 112.65 | 12.25 | 103.76 | 3.39 |
| $PtBr_4$ | 150.62 | 150.94 | 0.21 | 129.70 | 13.89 |
| $PtCl_2$ | 75.40 | 74.45 | 1.27 | 77.82 | 3.21 |
| $PtCl_3$ | 121.34 | 109.05 | 10.13 | 103.76 | 14.49 |
| $PtCl_4$ | 146.44 | 146.13 | 0.22 | 129.70 | 11.43 |
| $Pu_2O_3$ | 133.01 | 126.28 | 5.06 | 102.09 | 23.25 |
| $PuBr_3$ | 107.86 | 113.08 | 4.84 | 103.76 | 3.80 |
| $PuCl_3$ | 102.86 | 109.48 | 6.43 | 103.76 | 0.88 |
| $PuF_3$ | 92.63 | 100.98 | 9.01 | 88.70 | 4.25 |
| $PuF_4$ | 116.18 | 116.36 | 0.16 | 109.62 | 5.64 |
| $PuF_6$ | 137.52 | 144.44 | 5.03 | 151.46 | 10.13 |
| $PuO_2$ | 66.28 | 65.91 | 0.56 | 59.41 | 10.36 |
| PuOBr | 87.79 | 79.79 | 9.12 | 68.62 | 21.84 |
| PuOCl | 83.64 | 78.58 | 6.05 | 68.62 | 17.96 |
| $Rb_2CO_3$ | 117.67 | 118.37 | 0.59 | 109.62 | 6.84 |
| $Rb_2O$ | 73.97 | 78.65 | 6.34 | 68.62 | 7.23 |
| $Rb_2Si_2O_5$ | 170.66 | 167.01 | 2.14 | 167.36 | 1.94 |
| $Rb_2Si_4O_9$ | 270.85 | 255.38 | 5.71 | 266.10 | 1.75 |
| $Rb_2SiO_3$ | 117.40 | 122.83 | 4.63 | 117.99 | 0.50 |
| $Rb_2SO_4$ | 133.96 | 135.47 | 1.13 | 141.42 | 5.56 |
| RbBr | 52.55 | 55.97 | 6.52 | 51.88 | 1.27 |
| RbCl | 51.36 | 54.77 | 6.65 | 51.88 | 1.02 |
| RbF | 50.47 | 51.94 | 2.92 | 46.86 | 7.14 |
| RbI | 51.45 | 56.71 | 10.23 | 51.88 | 0.84 |
| $ReAgO_4$ | 116.24 | 106.69 | 8.22 | 92.88 | 20.09 |
| $ReCl_3$ | 92.22 | 80.79 | 12.39 | 77.82 | 15.61 |
| $ReNH_4O_4$ | 149.71 | 159.27 | 6.38 | 157.32 | 5.08 |
| $ReO_2$ | 56.58 | 56.58 | 0.00 | 59.41 | 5.01 |
| $ReO_3$ | 72.77 | 72.77 | 0.00 | 76.15 | 4.64 |
| $Rh_2O_3$ | 103.99 | 101.47 | 2.42 | 102.09 | 1.82 |

| COMPOUNDS | $C_{p,literature}^{298}$ | $C_{p,predicted}^{298}$ | % Error | $C_{p,Kopp's\ rule}^{298}$ | % Error |
|---|---|---|---|---|---|
| $RhBr_3$ | 100.54 | 100.68 | 0.14 | 103.76 | 3.21 |
| $RhCl_3$ | 92.18 | 97.07 | 5.31 | 103.76 | 12.57 |
| $RuCl_3$ | 115.06 | 115.06 | 0.00 | 103.76 | 9.82 |
| $RuO_2$ | 52.66 | 52.66 | 0.00 | 59.41 | 12.81 |
| $Sb_2(SO_4)_3$ | 275.44 | 278.59 | 1.15 | 320.49 | 16.36 |
| $SbBr_3$ | 112.97 | 104.01 | 7.93 | 103.76 | 8.15 |
| $SbCl_3$ | 107.50 | 100.40 | 6.61 | 103.76 | 3.48 |
| $SbF_3$ | 90.29 | 91.90 | 1.79 | 88.70 | 1.76 |
| $SbI_3$ | 98.08 | 106.22 | 8.30 | 103.76 | 5.79 |
| $Sc_2O_3$ | 93.93 | 93.08 | 0.91 | 102.09 | 8.68 |
| $ScBr_3$ | 95.34 | 96.49 | 1.20 | 103.76 | 8.84 |
| $ScCl_3$ | 92.04 | 92.88 | 0.91 | 103.76 | 12.74 |
| $ScF_3$ | 84.67 | 84.38 | 0.34 | 88.70 | 4.76 |
| $Se_2O_5$ | 127.33 | 127.33 | 0.00 | 135.56 | 6.46 |
| $SeCl_4$ | 133.90 | 118.00 | 11.87 | 129.70 | 3.13 |
| $SeO_3$ | 75.69 | 65.38 | 13.63 | 76.15 | 0.60 |
| $SiI_4$ | 108.03 | 113.73 | 5.27 | 119.66 | 10.77 |
| $SiO_2$ | 44.41 | 44.18 | 0.52 | 49.37 | 11.17 |
| $Sm_2O_3$ | 115.80 | 116.03 | 0.19 | 102.09 | 11.84 |
| $Sm_2O_3.2ZrO_2$ | 224.23 | 228.13 | 1.74 | 220.92 | 1.48 |
| $SmCl_2$ | 82.39 | 82.39 | 0.00 | 77.82 | 5.54 |
| $SmCl_3$ | 99.52 | 104.35 | 4.86 | 103.76 | 4.27 |
| $SmF_3$ | 106.75 | 95.85 | 10.21 | 88.70 | 16.91 |
| SmOCl | 71.10 | 73.46 | 3.31 | 68.62 | 3.50 |
| SmOF | 69.56 | 70.63 | 1.54 | 63.60 | 8.57 |
| $SnBr_2$ | 78.97 | 78.53 | 0.56 | 77.82 | 1.46 |
| $SnCl_2$ | 78.02 | 76.13 | 2.43 | 77.82 | 0.26 |
| $SnF_2$ | 72.39 | 70.46 | 2.66 | 67.78 | 6.37 |
| $SnI_2$ | 79.02 | 80.01 | 1.25 | 77.82 | 1.51 |
| $SnI_4$ | 131.96 | 137.75 | 4.39 | 129.70 | 1.71 |
| SnO | 47.76 | 45.24 | 5.28 | 42.68 | 10.65 |
| $SnO_2$ | 52.58 | 52.58 | 0.00 | 59.41 | 13.00 |
| $Sr_2SiO_4$ | 130.75 | 130.09 | 0.50 | 134.72 | 3.04 |
| $Sr_2TiO_4$ | 143.66 | 144.02 | 0.26 | 144.77 | 0.77 |
| $SrBr_2$ | 76.86 | 76.25 | 0.79 | 77.82 | 1.26 |
| $SrCl_2$ | 75.60 | 73.85 | 2.32 | 77.82 | 2.94 |
| $SrF_2$ | 69.92 | 68.18 | 2.48 | 67.78 | 3.06 |
| $SrHfO_3$ | 103.91 | 102.59 | 1.27 | 102.09 | 1.75 |

| COMPOUNDS | $C_{p,Literature}^{298}$ | $C_{p,predicted}^{298}$ | % Error | $C_{p,Kopp's\ rule}^{298}$ | % Error |
|---|---|---|---|---|---|
| $SrI_2$ | 77.96 | 77.73 | 0.30 | 77.82 | 0.18 |
| $SrMoO_4$ | 117.03 | 117.77 | 0.64 | 118.83 | 1.54 |
| SrO | 45.49 | 42.95 | 5.57 | 42.68 | 6.18 |
| $SrO_2$ | 79.35 | 79.35 | 0.00 | 59.41 | 25.12 |
| $SrSiO_3$ | 87.05 | 87.14 | 0.10 | 92.05 | 5.74 |
| $SrTiO_3$ | 99.04 | 101.07 | 2.05 | 102.09 | 3.08 |
| $SrZrO_3$ | 100.79 | 99.01 | 1.77 | 102.09 | 1.29 |
| $Ta_2O_5$ | 131.44 | 139.07 | 5.80 | 135.56 | 3.14 |
| $TaBr_5$ | 155.69 | 152.77 | 1.87 | 155.64 | 0.03 |
| $TaCl_3$ | 93.06 | 93.06 | 0.00 | 103.76 | 11.51 |
| $TaCl_4$ | 119.81 | 119.81 | 0.00 | 129.70 | 8.26 |
| $TaCl_5$ | 147.90 | 146.76 | 0.77 | 155.64 | 5.24 |
| $TaF_5$ | 133.89 | 132.60 | 0.96 | 130.54 | 2.50 |
| $TaI_5$ | 156.21 | 156.46 | 0.16 | 155.64 | 0.36 |
| $TaOCl_3$ | 119.81 | 115.87 | 3.29 | 120.50 | 0.57 |
| $Tb_2O_3$ | 115.03 | 108.90 | 5.33 | 102.09 | 11.25 |
| $TbCl_3$ | 97.47 | 100.79 | 3.40 | 103.76 | 6.45 |
| $TbF_3$ | 92.94 | 92.29 | 0.70 | 88.70 | 4.56 |
| $TbI_3$ | 97.89 | 106.61 | 8.90 | 103.76 | 5.99 |
| $TbO_2$ | 61.52 | 61.52 | 0.00 | 59.41 | 3.42 |
| $TcO_2$ | 55.65 | 55.65 | 0.00 | 59.41 | 6.75 |
| $TcO_3$ | 107.95 | 107.95 | 0.00 | 76.15 | 29.46 |
| $TeCl_4$ | 138.49 | 132.07 | 4.63 | 129.70 | 6.34 |
| $TeO_2$ | 63.88 | 70.29 | 10.04 | 59.41 | 6.99 |
| $Th_2N_2O$ | 104.77 | 104.77 | 0.00 | 120.50 | 15.01 |
| $ThBr_4$ | 125.17 | 128.15 | 2.38 | 129.70 | 3.62 |
| $ThCl_4$ | 120.28 | 123.34 | 2.55 | 129.70 | 7.83 |
| $ThF_4$ | 110.53 | 112.01 | 1.34 | 109.62 | 0.82 |
| $ThI_4$ | 145.98 | 131.11 | 10.19 | 129.70 | 11.15 |
| $ThO_2$ | 61.80 | 61.56 | 0.39 | 59.41 | 3.87 |
| $ThOBr_2$ | 93.46 | 94.86 | 1.50 | 94.56 | 1.18 |
| $ThOCl_2$ | 91.00 | 92.45 | 1.59 | 94.56 | 3.91 |
| $ThOF_2$ | 86.24 | 86.79 | 0.63 | 84.52 | 2.00 |
| $ThOI_2$ | 103.82 | 96.33 | 7.21 | 94.56 | 8.92 |
| $Ti_2O_3$ | 101.78 | 103.97 | 2.16 | 102.09 | 0.31 |
| $TiBr_2$ | 78.73 | 77.24 | 1.89 | 77.82 | 1.15 |
| $TiBr_3$ | 100.03 | 101.93 | 1.91 | 103.76 | 3.74 |
| $TiBr_4$ | 131.48 | 124.71 | 5.15 | 129.70 | 1.35 |

| COMPOUNDS | $C_{p,Literature}^{298}$ | $C_{p,predicted}^{298}$ | % Error | $C_{p,Kopp's\ rule}^{298}$ | % Error |
|---|---|---|---|---|---|
| $TiCl_2$ | 69.84 | 74.84 | 7.16 | 77.82 | 11.44 |
| $TiCl_3$ | 97.07 | 98.32 | 1.29 | 103.76 | 6.90 |
| $TiF_3$ | 91.63 | 89.83 | 1.97 | 88.70 | 3.20 |
| $TiF_4$ | 114.19 | 108.57 | 4.92 | 109.62 | 4.00 |
| $TiI_2$ | 86.24 | 78.72 | 8.72 | 77.82 | 9.76 |
| $TiI_3$ | 116.79 | 104.15 | 10.83 | 103.76 | 11.16 |
| $TiI_4$ | 125.62 | 127.66 | 1.63 | 129.70 | 3.25 |
| TiO | 39.93 | 43.94 | 10.04 | 42.68 | 6.87 |
| $TiO_2$ | 55.28 | 58.11 | 5.12 | 59.41 | 7.47 |
| $Tl_2O$ | 78.84 | 78.14 | 0.89 | 68.62 | 12.97 |
| $Tl_2O_3$ | 105.42 | 107.58 | 2.04 | 102.09 | 3.16 |
| $Tl_2SO_4$ | 137.82 | 134.96 | 2.08 | 141.42 | 2.61 |
| TlBr | 50.47 | 55.72 | 10.39 | 51.88 | 2.79 |
| TlCl | 50.93 | 54.52 | 7.04 | 51.88 | 1.87 |
| TlF | 53.38 | 51.68 | 3.18 | 46.86 | 12.21 |
| TlI | 52.51 | 48.20 | 8.20 | 51.88 | 1.20 |
| $Tm_2O_3$ | 116.71 | 114.99 | 1.48 | 102.09 | 12.53 |
| $TmCl_3$ | 97.67 | 103.83 | 6.31 | 103.76 | 6.23 |
| $TmF_3$ | 94.97 | 95.34 | 0.38 | 88.70 | 6.60 |
| $UBr_3$ | 108.73 | 107.96 | 0.71 | 103.76 | 4.57 |
| $UBr_4$ | 128.11 | 129.74 | 1.27 | 129.70 | 1.24 |
| $UCl_3$ | 102.52 | 104.35 | 1.79 | 103.76 | 1.21 |
| $UCl_4$ | 120.77 | 124.93 | 3.44 | 129.70 | 7.40 |
| $UCl_5$ | 144.57 | 146.12 | 1.08 | 155.64 | 7.66 |
| $UCl_6$ | 175.53 | 179.32 | 2.16 | 181.59 | 3.45 |
| $UF_3$ | 95.08 | 95.86 | 0.82 | 88.70 | 6.71 |
| $UF_4$ | 116.01 | 113.60 | 2.08 | 109.62 | 5.51 |
| $UF_5$ | 132.30 | 131.96 | 0.26 | 130.54 | 1.33 |
| $UF_6$ | 167.43 | 162.33 | 3.05 | 151.46 | 9.54 |
| $UI_3$ | 112.02 | 110.18 | 1.65 | 103.76 | 7.37 |
| $UI_4$ | 134.43 | 132.69 | 1.30 | 129.70 | 3.52 |
| $UO_2$ | 63.57 | 63.14 | 0.68 | 59.41 | 6.54 |
| $UO_2F_2$ | 103.04 | 111.88 | 8.58 | 101.25 | 1.73 |
| $UO_2SO_4$ | 144.88 | 143.47 | 0.97 | 148.95 | 2.81 |
| $UO_3$ | 81.16 | 86.65 | 6.76 | 76.15 | 6.18 |
| $UO_3.2H_2O$ | 154.52 | 160.65 | 3.97 | 148.11 | 4.15 |
| $UO_3.H_2O$ | 117.46 | 123.65 | 5.27 | 112.13 | 4.54 |
| $UOBr_2$ | 97.88 | 96.44 | 1.47 | 94.56 | 3.40 |

| COMPOUNDS | $C_{p,Literature}^{298}$ | $C_{p,predicted}^{298}$ | % Error | $C_{p,Kopp's\ rule}^{298}$ | % Error |
|---|---|---|---|---|---|
| $UOBr_3$ | 121.11 | 118.84 | 1.87 | 120.50 | 0.50 |
| $UOCl_2$ | 94.97 | 94.03 | 0.98 | 94.56 | 0.43 |
| $UOCl_3$ | 115.40 | 115.23 | 0.15 | 120.50 | 4.42 |
| $V_2O_5$ | 127.33 | 127.28 | 0.04 | 135.56 | 6.46 |
| $VBr_2$ | 77.38 | 74.20 | 4.11 | 77.82 | 0.57 |
| $VBr_3$ | 101.65 | 99.08 | 2.52 | 103.76 | 2.08 |
| $VCl_2$ | 71.86 | 71.79 | 0.09 | 77.82 | 8.29 |
| $VCl_3$ | 93.17 | 95.47 | 2.47 | 103.76 | 11.37 |
| $VF_3$ | 89.84 | 86.98 | 3.19 | 88.70 | 1.27 |
| $VF_4$ | 107.03 | 113.14 | 5.71 | 109.62 | 2.42 |
| $VI_2$ | 74.80 | 75.68 | 1.17 | 77.82 | 4.04 |
| $VI_3$ | 99.73 | 101.30 | 1.57 | 103.76 | 4.04 |
| VO | 38.53 | 40.90 | 6.17 | 42.68 | 10.77 |
| $VO_2$ | 56.87 | 62.69 | 10.23 | 59.41 | 4.48 |
| $VOSO_4$ | 131.44 | 119.51 | 9.07 | 132.21 | 0.59 |
| $W(CO)_6$ | 242.65 | 243.67 | 0.42 | 171.54 | 29.30 |
| $WBr_5$ | 155.47 | 158.55 | 1.98 | 155.64 | 0.11 |
| $WBr_6$ | 181.40 | 177.13 | 2.35 | 181.59 | 0.10 |
| $WCl_2$ | 77.81 | 77.81 | 0.00 | 77.82 | 0.02 |
| $WCl_2O_2$ | 104.35 | 108.13 | 3.63 | 111.29 | 6.66 |
| $WCl_4$ | 129.72 | 124.16 | 4.29 | 129.70 | 0.01 |
| $WCl_5$ | 155.61 | 152.53 | 1.98 | 155.64 | 0.02 |
| $WCl_6$ | 175.40 | 169.91 | 3.13 | 181.59 | 3.53 |
| $WH_2O_4$ | 104.08 | 100.21 | 3.71 | 92.88 | 10.75 |
| $WO_2$ | 56.82 | 62.38 | 9.79 | 59.41 | 4.57 |
| $WO_3$ | 72.78 | 77.24 | 6.12 | 76.15 | 4.62 |
| $WOCl_4$ | 146.24 | 139.02 | 4.94 | 146.44 | 0.13 |
| $Y_2O_3$ | 102.49 | 100.54 | 1.90 | 102.09 | 0.39 |
| $Yb_2O_3$ | 115.34 | 112.25 | 2.68 | 102.09 | 11.49 |
| $YbCl_2$ | 74.22 | 74.22 | 0.00 | 77.82 | 4.85 |
| $YbCl_3$ | 95.34 | 102.46 | 7.47 | 103.76 | 8.83 |
| $YbF_3$ | 94.56 | 93.96 | 0.63 | 88.70 | 6.20 |
| $YCl_3$ | 92.01 | 96.61 | 4.99 | 103.76 | 12.77 |
| $YF_3$ | 95.24 | 88.11 | 7.48 | 88.70 | 6.86 |
| $YI_3$ | 96.00 | 102.43 | 6.69 | 103.76 | 8.08 |
| $Zn_2SiO_4$ | 121.79 | 124.12 | 1.91 | 134.72 | 10.62 |
| $Zn_2TiO_4$ | 137.29 | 138.05 | 0.55 | 144.77 | 5.45 |
| $Zn_3O(SO_4)_2$ | 238.35 | 233.55 | 2.01 | 273.63 | 14.81 |

| COMPOUNDS | $C_{p,Literature}^{298}$ | $C_{p,predicted}^{298}$ | % Error | $C_{p,Kopp's\ rule}^{298}$ | % Error |
|---|---|---|---|---|---|
| $ZnAl_2O_4$ | 119.31 | 117.50 | 1.52 | 144.77 | 21.33 |
| $ZnBr_2$ | 65.69 | 73.26 | 11.54 | 77.82 | 18.48 |
| $ZnCl_2$ | 71.05 | 70.86 | 0.27 | 77.82 | 9.53 |
| $ZnCO_3$ | 80.06 | 79.69 | 0.46 | 83.68 | 4.53 |
| $ZnCr_2O_4$ | 143.33 | 143.74 | 0.28 | 144.77 | 1.00 |
| $ZnF_2$ | 65.61 | 65.19 | 0.64 | 67.78 | 3.31 |
| $ZnFe_2O_4$ | 137.27 | 146.84 | 6.97 | 144.77 | 5.46 |
| $ZnI_2$ | 74.43 | 74.74 | 0.42 | 77.82 | 4.56 |
| ZnO | 41.06 | 39.97 | 2.66 | 42.68 | 3.94 |
| $ZnSeO_3$ | 93.66 | 96.19 | 2.71 | 102.09 | 9.00 |
| $ZnWO_4$ | 125.50 | 117.21 | 6.61 | 118.83 | 5.32 |
| $ZrBr_2$ | 86.71 | 82.09 | 5.33 | 77.82 | 10.25 |
| $ZrBr_3$ | 99.47 | 99.30 | 0.17 | 103.76 | 4.32 |
| $ZrBr_4$ | 124.80 | 122.64 | 1.72 | 129.70 | 3.93 |
| $ZrCl_2$ | 72.60 | 79.69 | 9.76 | 77.82 | 7.19 |
| $ZrCl_3$ | 96.20 | 95.69 | 0.53 | 103.76 | 7.86 |
| $ZrCl_4$ | 119.83 | 117.83 | 1.67 | 129.70 | 8.24 |
| $ZrF_2$ | 65.93 | 74.03 | 12.29 | 67.78 | 2.81 |
| $ZrF_3$ | 83.66 | 87.19 | 4.23 | 88.70 | 6.03 |
| $ZrF_4$ | 102.98 | 106.51 | 3.43 | 109.62 | 6.45 |
| $ZrI_2$ | 94.14 | 83.57 | 11.23 | 77.82 | 17.33 |
| $ZrI_3$ | 104.37 | 101.51 | 2.73 | 103.76 | 0.58 |
| $ZrI_4$ | 125.11 | 125.60 | 0.39 | 129.70 | 3.67 |
| $ZrO_2$ | 56.19 | 56.05 | 0.24 | 59.41 | 5.74 |
| $ZrSiO_4$ | 98.54 | 100.23 | 1.72 | 108.78 | 10.40 |