

Open Notebook Science Challenge  
Solubilities  
of  
Organic Compounds  
in  
Organic Solvents

Compiled and Measured by:

Jean-Claude Bradley, Associate Professor of Chemistry at Drexel University  
Cameron Neylon, Senior Scientist at the ISIS Pulsed Neutron Source, Rutherford Appleton Laboratory  
and Lecturer in Chemical Biology at the School of Chemistry at the University of Southampton  
Rajarshi Guha, Research Scientist at the NIH Chemical Genomics Center  
Antony Williams, Vice President of Strategic Development, ChemSpider at the Royal Society of Chemistry  
Bill Hooker, Postdoctoral Researcher in Molecular Biology  
Andrew Lang, Professor of Mathematics at Oral Roberts University  
Brent Friesen, Associate Professor of Chemistry at Dominican University

and

Tim Bohinski, David Bulger, Matthew Federici, Jenny Hale, Jenna Mancinelli, Khalid Mirza, Marshall Moritz, Daniel Rein, Cedric Tchakounte, and Hai Truong



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# Preface

## The Open Notebook Science Solubility Challenge

Solubility is an important consideration for many chemistry applications. Synthetic chemists usually use a solvent to perform reactions and knowledge of the solubility of the starting materials or products can be very useful to pick an appropriate solvent. Analytical chemists can use solubility to design separation techniques and factor in dynamic range considerations. Physical chemists can create and evaluate their models of how molecules interact in the solubilization and precipitation processes.

Solubility data can be obtained from a variety of online and offline sources. As with all chemical data, it can be a challenge to evaluate reported measurements. Some databases offer no references while others provide citations to peer reviewed journal articles. Given the choice, more weight is generally given to the latter. This is reasonable in most cases because more information about the purity of compounds and the methods used are available in peer-reviewed articles.

However, the information for how a specific measurement was obtained within a journal article is not generally provided. General methods are provided but the raw data for a specific measurement are typically not published. Peer review is not intended to validate individual measurements - its function is to ensure that the authors made appropriate conclusions based on their processed datasets and the state of knowledge in the field.

The Open Notebook Science Challenge was initiated in the fall of 2008 as the result of a discussion on a train in the UK between Jean-Claude Bradley and Cameron Neylon.[1,2] The concept was very simple: create a crowdsourcing opportunity for the chemistry community to contribute solubility measurements under Open Notebook Science conditions. This method of publication entails providing immediate public access to the chemist's laboratory notebook, as well as all raw data used to compute the measurements.[3,4]

On Sept 3, 2008 the first ONSC measurements were recorded by Bradley and Neylon at the University of Southampton in Neylon's laboratory.[5] The project was soon sponsored by Submeta, offering ten \$500 awards for students in the US or the UK who best recorded how they performed their experiments.[6] Furthermore, the first 3 winners also received one year subscriptions to Nature magazine, thanks to a sponsorship from the Nature Publishing Group.[7] Sigma-Aldrich supported the contest by donating chemicals upon request.[8]

Students were evaluated by a group of judges who convened once a month to deliberate the next award. Judges also provided feedback to the students by commenting on their lab notebook pages directly on the wiki. Their expertise ranged from chemistry to mathematics, spectroscopy and molecular biology.

### Techniques

Participants in the ONS Challenge were not required to use a specific method to measure solubility - although they were required to properly document their experiments and analyses. Due to its simplicity, most measurements in the past year were made using the SAMS NMR technique, requiring no volume measurement or calibration curves.[9] Two assumptions are made with this method. The first is that the volume of solute and solvent are additive, with the error becoming negligible at low solubility values. The second is that NMR integration values are proportional to the amount of solvent and solute. Some deviations from this have been observed for default NMR parameters and in later experiments long relaxation times are introduced into the protocol (D1 = 50s).[10]

### Data Curation

Since an Open Notebook approach is used in this work, those interested in the validity of the measurements can assess the methods used - both for the preparation of saturated solutions and the raw data from the measurements. Over time, values in the database are likely to improve and possibly some errors may be uncovered and corrected. However, on the whole, we feel that the values provided in this work should be of use to chemists trying to gain an appreciation of solubility for most applications. This is especially the case for values that are not obtainable from any other source.

When clearly erroneous data points are discovered, they are flagged in the database as "DONOTUSE". This way interfaces with the dataset can ignore these values while allowing anyone to investigate why the data points were flagged. This might happen when early experiments did not allow for sufficient mixing or NMR D1 relaxation times were long enough to fully integrate peaks of interest. Out of 681 reported measurements, 51 are currently marked in this way. A shared Google Spreadsheet is used to collect and curate the dataset. This allows easy data entry while providing a simple way to interrogate the database for visualization applications via the Google API.[11]

### Literature data and format conversions

An additional 400 solubility measurements from the literature are included in the database. These generally correspond to compounds that are structurally identical or similar to the compounds measured by the ONS Challenge participants. These values are averaged in with the values from the participants, with appropriate references provided. In order to compare values, conversions from molar fraction or g solute/100g solvent to molarity were made by assuming that the volumes are additive and obtaining the density of the solutes in most cases from the predicted values in ChemSpider.[12]

For the convenience of chemists with diverse applications, all three formats are provided. For the cases where solutes are miscible with the solvent, the molarity reported is simply the solute's density. The practical interpretation of this is that solutions of any molarity below the solute's density can be prepared.

In the process of converting units and averaging heterogeneous data sources, no attempt has been made to track significant figures. Those interested in any information about the precision of measurements should consult each individual data source.

This may not be an easy task for measurements only carried out once and where factors such as the quality of spectral peaks and baselines are not optimal.

This collection will be most valuable for those who do not require highly precise measurements for their applications. For example, synthetic chemists can easily use rough estimates of solubility to select appropriate solvents for a reaction. In any case, one would be wise to consider all measurements as provisional, regardless of the source. As more data are collected, subsequent editions of this book will adjust values accordingly.

## Searching the database

The values in this database can be accessed and filtered in various ways. More information is available at the ONS Challenge wiki[13] and Chapter 16 of the book "Beautiful Data".[14]

## Database version

Archived as Excel Spreadsheet by WebCite on December 11, 2009.[15]

## References

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- [12] ChemSpider database <http://www.chemspider.com>
- [13] ONS Challenge List of Experiments Page <http://onschallenge.wikispaces.com/list+of+experiments>
- [14] Bradley, J.-C.; Guha, R.; Lang, A.S.I.D.; Lindenbaum, P; Neylon, C.; Williams, A.J. & Willighagen, E. [Chapter 16: Beautifying Data in the Real World](#) from Beautiful Data. O'Reilly Media, Eds: Segaran, T. & Hammerbacher, J. (2009)
- [15] Bradley, Jean-Claude; Lang Andrew. Solubilities Summary Sheet. Open Notebook Science Challenge. 2009-12-11. URL:<http://spreadsheets.google.com/pub?key=plwwufp30hfq0udnEmRD1aQ&output=xls>. Accessed: 2009-12-11. (Archived byWebCite® at <http://www.webcitation.org/5ix5ry3BV>)

# Judges



**Jean-Claude Bradley** is an Associate Professor of Chemistry and E-Learning Coordinator for the College of Arts and Sciences at Drexel University. He leads the UsefulChem project, an initiative started in the summer of 2005 to make the scientific process as transparent as possible by publishing all research work in real time to a collection of public blogs, wikis and other web pages. Jean-Claude coined the term Open Notebook Science to distinguish this approach from other more restricted forms of Open Science. Jean-Claude teaches undergraduate organic chemistry courses with most content freely available on public blogs, wikis, games, Second Life and audio and video podcasts. He has a Ph.D. in organic chemistry and has published articles and obtained patents in the areas of synthetic and mechanistic chemistry, gene therapy, nanotechnology and scientific knowledge management. <http://usefulchem.blogspot.com>



**Cameron Neylon** is a biophysicist who has always worked in interdisciplinary areas and is an advocate of open research practice and improved data management. He currently works as Senior Scientist in Biomolecular Sciences at the ISIS Neutron Scattering facility at the Science and Technology Facilities Council (STFC). Along with his work in structural biology and biophysics his research and writing focuses on the interface of web technology with science and the successful (and unsuccessful) application of generic and specially designed tools in the academic research environment. He is a founder member of the Open Knowledge Foundation Science Working Group and writes regularly on Open Research at his blog, Science in the Open.

<http://blog.openwetware.org/scienceintheopen>



**Rajarshi Guha** is a Research Scientist at the NIH Chemical Genomics Center (NCGC). At the NCGC he is involved in cheminformatics methodology and software development for various aspects of high throughput screening for small molecules and RNAi. His research makes extensive use of statistical methods and has been applied to a variety of biological systems. Along with algorithm development, he is extensively involved in cheminformatics software development, including development of toolkits, web services and integration of these into distributed infrastructures. As a believer in Open Source and Open Data, much of his research and software is available under Open Source licenses.

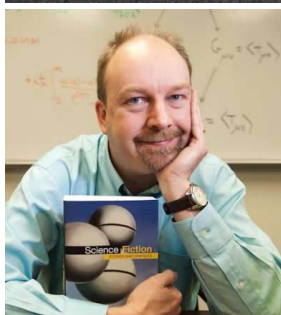
<http://blog.rguha.net>



Antony Williams is the host of ChemSpider, the online chemistry portal leading the charge towards open and collaborative chemistry. ChemSpider provides access to over 23million unique chemical entities sourced from almost 300 data sources and provides a platform for community based depositions and curation to clean up internet-based chemistry. Antony spent over a decade in the commercial scientific software business as Chief Science Officer for a Cheminformatics software company and during his tenure over saw their product development, marketing and sales teams. He is an accomplished NMR spectroscopist with over 100 peer-reviewed publications. During his career he was the NMR Technology Leader for the Eastman-Kodak company and has worked in both academia and national government research institutions. He has recently taken his passion for providing access to chemistry related information and software services to the masses by hosting the ChemSpider service. <http://www.chemspider.com/blog/>



**Bill Hooker** is a molecular biologist by trade and has worked on G protein signaling, PCR diagnostics, anti-schistosome vaccines, HIV replication and molecular mechanisms of cancer. He serves as an associate editor on the innovative Open Access journal BioMed Central Research Notes and as a member of the advisory board of the Berglund Center for Internet Studies. He is currently the R&D team leader at a small biotech company in Portland, OR. He has never had an idea that couldn't be improved by sharing it with as many people as possible, and doesn't believe that anyone else has, either. He is particularly interested in extending the "open" ethos of Open Source software and Open Access publishing to all aspects of science, from raw data to hypothesis testing by way of distributed, collaborative effort. <http://www.sennoma.net>



**Andrew Lang** is a Professor of Mathematics at Oral Roberts University. His PhD training is in the area of quantum field theory in curved spacetime. While remaining active in this area he has always enjoyed working collaboratively on interdisciplinary projects ranging from modeling basketball free throws to the stability of spinning spacecraft under thrust. His interests include the relationship between science and science fiction and the epistemological differences between teleology and metaphysical naturalism. As a result of being a judge for the Open Notebook Science Challenge he has developed an appreciation for openness in science, multi-dimensional data visualization and cheminformatics. [http://webapps.oru.edu/new\\_php/blog/index.php?user\\_id=23](http://webapps.oru.edu/new_php/blog/index.php?user_id=23)

## Educational Partners



**J. Brent Friesen from Dominican University** incorporated the Open Notebook Science Solubility Challenge into his Sophomore Organic Chemistry laboratory course in January 2009. He has been a professor in the natural science department at Dominican University since 1999. He regularly teaches Organic Chemistry (lecture and laboratory), Biochemistry, Introduction to Organic Chemistry, Chemistry of Natural Products, and Forensic Chemistry. His research focuses on the automation of countercurrent separation technology, anti-tuberculosis compounds, and interactions with Reichardt's Dye. Friesen has also done research with undergraduates on projects such as "Biorenewable Solvents for Countercurrent Chromatography" and "Used Coffee Grounds: A New Source of Biofuels." Friesen is a regular volunteer with the Oak Park Education Foundation's Global Village, a program matching scientists with elementary school classrooms. His recent articles include "Saying What You Mean: Teaching Mechanisms in Organic Chemistry" (Journal of Chemical Education) and "Countercurrent Separation of Natural Products" (Journal of Natural Products).

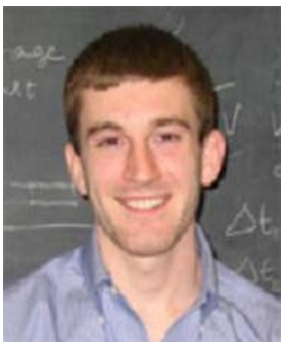
## Students



**Tim Bohinski (April 2009 Submeta Award winner)** is a senior at Drexel University majoring in chemistry, with a strong interest in organic and theoretical chemistry. He will be graduating with a B.S. in June 2010. He is currently performing undergraduate research in the theoretical/physical field, studying nanoparticle optics, specifically in the area of plasmoms. He plans to continue his studies at the doctorate level. Tim is also a member of the Drexel American Chemical Society and was a member of the Drexel Crew Team. In my spare time he enjoys the outdoors, staying fit, and homebrewing. LinkedIn profile: <http://www.linkedin.com/pub/timothy-bohinski/18/110/a7> Supervisor: Jean-Claude Bradley, Drexel



**David Bulger (February 2009 Submeta Award winner)** is a junior Chemistry major at Oral Roberts University in Tulsa, OK. Since freshman year, he has been involved in research ranging from water purity, red tide in Second Life, collaboration between water utilities and academia, NMR solubility determination and Sortase A inhibition. After his undergraduate degree, he plans to pursue an M.D. or M.D./Ph.D. [http://biolab.isis.rl.ac.uk/david\\_bulger](http://biolab.isis.rl.ac.uk/david_bulger). Supervisor: Robert Stewart, Oral Roberts University



**Matthew Federici (June 2009 Submeta Award winner)** graduated from the University of Virginia in 2008. After receiving the Naval ROTC Tweeddale Scholarship Award in 2004, Matthew studied naval nuclear engineering and interned on the USS Alexandria. As a varsity student athlete, he doubled majored in mechanical engineering as well as aerospace engineering. Matthew spent his senior year at UVa studying biomechanics under Dr. Pradip Sheth. His undergraduate academic career finished by winning the Cyrus Society Award, given to a select few of student athletes with outstanding academic performance and community service. Matthew is pursuing his PhD in Mechanical Engineering under Dr. Minjun Kim at Drexel University. As a GAANN fellow, he is currently investigating biomimetics and drug delivery systems. Matthew plans to attend medical school following the completion of his dissertation. Website: <http://microfluidics.tripod.com/> Supervisor: Jean-Claude Bradley, Drexel



**Jennifer (Jenny) Hale (December 2008 Submeta Award winner)** gained a BSc in Chemistry with Pharmacology from the University of Southampton, UK, in 2004. Following her degree she spent 15 months working on the synthesis of phosphoramidites before taking up a PhD in the department of chemical biology in 2006. Jenny's area of research for her PhD has been the directed evolution of a beta-glucuronidase into a beta-galactosidase via neutral drift, a phenomenon found in natural evolution that has only recently begun to be explored in laboratory evolution. Additionally, her research has been used in the development and testing of an electronic laboratory notebook in the form of a blog: LaBLog ([http://blogs.chem.soton.ac.uk/neutral\\_drift](http://blogs.chem.soton.ac.uk/neutral_drift)) as well as wider investigations into Open Notebook Science. Outside of the laboratory, Jenny is a keen ballroom and latin dancer and spent a year as president of the Southampton University Ballroom and Latin Dance Society, as well as competing in numerous university dancesport competitions.  
**Supervisor: Cameron Neylon, Southampton**



**Jenna Mancinelli (September 2009 Submeta Award winner)** is currently a junior at Drexel University, studying Biology. She is particularly interested in human physiology and its relation to clinical medicine. She hopes to attend medical school following her graduation from Drexel University. In her spare time, Jenna enjoys going to concerts, studying Italian and experimenting with her culinary skills. **Supervisor: Jean-Claude Bradley, Drexel**



**Khalid Baig Mirza (January 2009 Submeta Award winner)** obtained a BSc in Chemistry and Biology from Osmania University, India. He earned an MS in Chemistry from Fairleigh Dickinson University at Madison, NJ in 2002. He is currently working towards a PhD at Drexel University under the guidance of Prof. Jean-Claude Bradley. His research focuses on the synthesis of potentially active anti-malarial diamides obtained from a Ugi reaction. His research is performed in the open as 'Open Notebook Science'. He enjoys gardening, cricket and keeping up to date on world affairs. **Supervisor: Jean-Claude Bradley, Drexel**



**Marshall Moritz (July 2009 Submeta Award winner)** is a junior at Syracuse University with a double major in chemistry and math. **Supervisor: Jean-Claude Bradley, Drexel**



**Daniel Rein (August 2009 Submeta Award winner)** is currently a student studying chemistry and biology at Drexel University. He plays guitar in Jazz Band and is passionate about music. For freshman year he studied physics at Northeastern. <http://www.linkedin.com/pub/daniel-rein/18/31a/72b> **Supervisor: Jean-Claude Bradley, Drexel**



**Cedric Tchakounte (March 2009 Submeta Award winner)** is a senior majoring in Biological Sciences & Biotechnology at Drexel University. He is a distinguished student, having received multiple Dean's List honors and the Who's Who Among Students in American Universities & Colleges award. He has also shown his dedication to community and service by being a mentor for Guided Youths. He enjoys performing research, because he believes it to be a cornerstone to learning true science. With his academic chapter as an undergraduate coming to an end, Cedric looks forward to what awaits. He plans on pursuing a career in medicine. **Supervisor: Jean-Claude Bradley, Drexel**

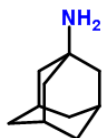




Hai Truong (December 2009 Submeta Award winner) is pursuing a BS in Chemistry at Drexel University from 2009. After graduating with honors from a high school for the Gifted in Vietnam, he came to the United States for college. In 2008, he attended Collin College in McKinney, TX. At Collin, he was a member of Phi Theta Kappa, an international honor society for two-year colleges. In 2009, he transferred to Drexel University with a Dean's Scholarship. Beside academic studies, Hai enjoys swimming and playing tennis. **Supervisor: Jean-Claude Bradley, Drexel**

## Solubilities

### 1-adamantylamine $C_{10}H_{17}N^{14}$



Compound Data			
Molecular weight	151.249	H bond acceptors	1 Rule of 5 violations 0
Compound type	amine	H bond donors	2 ACD/ALogP 2.22
Phase 25°C	solid	Rotatable bonds	1 Predicted density 1.066 g/cm <sup>3</sup>
SMILES	C1C2CC3CC1CC(C2)(C3)N		
InChIKey	DKNWSYNQZKUICI-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.82	0.05	17.99
methanol	0.36	0.02	7.62

### 1-octadecylamine $C_{18}H_{39}N^{69}$

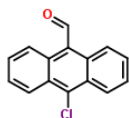


Compound Data			
Molecular weight	269.509	H bond acceptors	1 Rule of 5 violations 1
Compound type	amine	H bond donors	2 ACD/ALogP 8.37
Phase 25°C	solid	Rotatable bonds	17 Predicted density 0.818 g/cm <sup>3</sup>
SMILES	NCCCCCCCCCCCCCCCC		
InChIKey	REYJJPSVUYRZGE-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.08	0.00	2.96
ethanol	1.77	0.20	146.72
methanol	1.68	0.14	134.67
THF	1.68	0.23	112.18
toluene	1.34	0.20	74.24

### 10-chloro-9-anthraldehyde $C_{15}H_9ClO^{57}$

Compound Data			
Molecular weight	240.684	H bond acceptors	1 Rule of 5 violations 0



<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	4.7
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	1	<b>Predicted density</b>	1.327 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>O=Cc1c(ccc1)c(Cl)c3c2ccccc3</chem>				
<b>InChIKey</b>	SHYBXXMECBHHFH-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
ethanol	0.00	0.00	0.00
methanol	0.00	0.00	0.00
THF	0.08	0.01	2.16

## 2-(1,3-benzodioxol-5-yl)acetic acid C<sub>9</sub>H<sub>8</sub>O<sub>4</sub><sup>98, 82</sup>

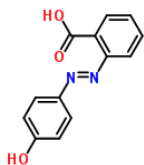
#### Compound Data

<b>Molecular weight</b>	180.157	<b>H bond acceptors</b>	4	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	1.37
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	2	<b>Predicted density</b>	1.406 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>O=C(O)Cc1ccc2OCOc2c1</chem>				
<b>InChIKey</b>	ODVLMCWNGKLROU-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
acetonitrile	0.67	0.04	17.68
DMSO	5.37	0.55	282.22
THF	2.73	0.25	83.68

## 2-(4-hydroxyphenyl-azo)benzoic acid C<sub>13</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub><sup>3, 32</sup>



#### Compound Data

<b>Molecular weight</b>	242.23	<b>H bond acceptors</b>	5	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	2	<b>ACD/ALogP</b>	3.72
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	4	<b>Predicted density</b>	1.3 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>Oc2ccc(N=Nc1ccccc1C(O)=O)cc2</chem>				
<b>InChIKey</b>	DWQOTEPNRWUDA-CCEZHUSRSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
ethanol	0.09	0.01	2.68
methanol	0.06	0.00	1.95
THF	0.55	0.05	16.42

## 2-chloro-5-nitrobenzaldehyde C<sub>7</sub>H<sub>4</sub>ClNO<sub>3</sub><sup>69, 105, 208, 33, 205</sup>



#### Compound Data

<b>Molecular weight</b>	185.565	<b>H bond acceptors</b>	4	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	2.5
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	2	<b>Predicted density</b>	1.485 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>O=Cc1cc(ccc1Cl)[N+](=O)[O-]</chem>				
<b>InChIKey</b>	VFVHWCKUHAEDMY-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	2.31	0.15	80.47
chloroform	2.9	0.27	56.27
DMSO	2.93	0.25	78.05
ethanol	*	*	*
methanol	*	*	*
THF	2.79	0.25	87.80
toluene	1.74	0.19	47.44

\* This aldehyde reacts with alcohols to form a hemiacetal.

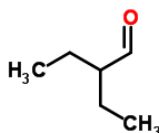
## 2-chloro-5-nitrobenzoic acid C<sub>7</sub>H<sub>4</sub>ClNO<sub>4</sub><sup>905</sup>



Compound Data			
<b>Molecular weight</b>	201.564	<b>H bond acceptors</b>	5 <b>Rule of 5 violations</b> 0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1 <b>ACD/ALogP</b> 2.02
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	2 <b>Predicted density</b> 1.602 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(O)c1cc(ccc1Cl)[N+](=O)[O-]		
<b>InChIKey</b>	QUEKGYQTRJVEQC-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.78	0.07	21.66
1-decanol	0.39	0.07	9.98
1-heptanol	0.54	0.08	14.24
1-hexanol	0.64	0.08	17.19
1-octanol	0.48	0.07	12.51
1-pentanol	0.74	0.08	20.28
1-propanol	0.95	0.08	27.36
2-butanol	0.91	0.09	25.86
2-methyl-1-propanol	0.63	0.06	17.22
2-methyl-2-propanol	1.21	0.12	35.78
2-pentanol	0.76	0.08	20.94
2-propanol	1.13	0.09	33.57
3-methyl-1-butanol	0.68	0.07	18.53
butyl acetate	0.46	0.06	11.11
dibutyl ether	0.1	0.02	2.62
diethyl ether	0.57	0.06	16.86
diisopropyl ether	0.19	0.03	5.18
ethanol	1.4	0.09	43.91
ethyl acetate	0.75	0.08	18.59
methyl acetate	0.89	0.08	22.25
pentyl acetate	0.43	0.06	10.39
THF	2.97	0.27	105.73

## 2-ethylbutyraldehyde C<sub>6</sub>H<sub>12</sub>O<sup>22</sup>

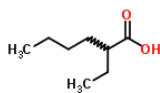


Compound Data			
<b>Molecular weight</b>	100.159	<b>H bond acceptors</b>	1 <b>Rule of 5 violations</b> 0
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0 <b>ACD/ALogP</b> 1.79
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	3 <b>Predicted density</b> 0.799 g/cm <sup>3</sup>
<b>SMILES</b>	O=CC(CC)CC		
<b>InChIKey</b>	UNNGUFMVYQJGTD-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.13	□	□

□ Solute is very soluble/miscible, conversion fail.

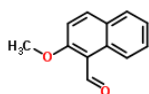
## 2-ethylhexanoic acid C<sub>8</sub>H<sub>16</sub>O<sub>2</sub><sup>22</sup>



Compound Data			
Molecular weight	144.211	H bond acceptors	2 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 2.72
Phase 25°C	liquid	Rotatable bonds	5 Predicted density 0.926 g/cm <sup>3</sup>
SMILES	O=C(O)C(CC)CCCC		
InChIKey	OBETXYAYXDNJHR-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	6.26	0.91	4777.15

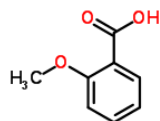
## 2-methoxy-1-naphthaldehyde C<sub>12</sub>H<sub>10</sub>O<sub>2</sub><sup>205</sup>



Compound Data			
Molecular weight	186.207	H bond acceptors	2 Rule of 5 violations 0
Compound type	aldehyde	H bond donors	0 ACD/ALogP 2.95
Phase 25°C	solid	Rotatable bonds	2 Predicted density 1.169 g/cm <sup>3</sup>
SMILES	O=Cc1c2c(ccc1OC)cccc2		
InChIKey	YIQLTKAOHRZOL-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	1.26	0.06	38.98

## 2-methoxybenzoic acid C<sub>8</sub>H<sub>8</sub>O<sub>3</sub><sup>905, 34</sup>

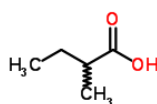


Compound Data			
Molecular weight	152.147	H bond acceptors	3 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 1.5
Phase 25°C	solid	Rotatable bonds	2 Predicted density 1.207 g/cm <sup>3</sup>
SMILES	O=C(O)c1ccccc1OC		
InChIKey	ILUJQPXNXACGAN-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.57	0.05	11.61
1-decanol	0.22	0.04	4.16
1-heptanol	0.34	0.05	6.59
1-hexanol	0.37	0.05	7.24
1-octanol	0.3	0.05	5.76
1-pentanol	0.47	0.05	9.37
1-propanol	0.76	0.06	16.09
1,4-dioxane	1.53	0.14	28.99
2-butanol	0.5	0.05	10.14
2-ethyl-1-hexanol	0.25	0.04	4.78
2-methyl-1-butanol	0.39	0.04	7.71
2-methyl-1-pentanol	0.35	0.04	6.84
2-methyl-1-propanol	0.41	0.04	8.21
2-methyl-2-propanol	0.53	0.05	10.75
2-pentanol	0.39	0.04	7.71
2-propanol	0.59	0.05	12.26

3-methyl-1-butanol	0.36	0.04	7.09
4-methyl-2-pentanol	0.32	0.04	6.26
butyl acetate	0.34	0.04	6.10
chloroform	0.47	0.04	5.01
dibutyl ether	0.04	0.01	0.78
diethyl ether	0.24	0.02	5.13
diisopropyl ether	0.06	0.01	1.21
ethanol	1.19	0.08	27.31
ethyl acetate	5.63	0.66	328.57
methanol	1.82	0.09	47.72
methyl acetate	0.86	0.07	16.16
pentyl acetate	0.26	0.04	4.64
propylene carbonate	0.99	0.13	14.28
THF	2.02	0.18	45.61

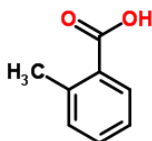
## 2-methyl butyric acid C<sub>5</sub>H<sub>10</sub>O<sub>2</sub><sup>22</sup>



Compound Data					
<b>Molecular weight</b>	102.132	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	1.13
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	2	<b>Predicted density</b>	0.962 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(O)C(C)CC				
<b>InChIKey</b>	WLAMNBDJUVNPJU-UHFFFAOYSA-N				

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
methanol	9.16	0.93	4515.12

## 2-methylbenzoic acid C<sub>8</sub>H<sub>8</sub>O<sub>2</sub><sup>905</sup>

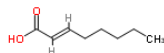


Compound Data					
<b>Molecular weight</b>	136.148	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	2.36
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	1	<b>Predicted density</b>	1.151 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(O)c1ccccc1C				
<b>InChIKey</b>	ZWLPBLYKEWSWPD-UHFFFAOYSA-N				

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
1-butanol	1.61	0.15	33.64
1-decanol	1.04	0.18	19.50
1-heptanol	1.28	0.18	25.04
1-hexanol	1.38	0.17	27.52
1-octanol	1.16	0.18	22.24
1-pentanol	1.49	0.16	30.37
1-propanol	1.77	0.14	38.34
1,4-dioxane	2.64	0.25	52.53
2-butanol	1.75	0.17	37.51
2-methyl-1-butanol	1.25	0.14	24.69
2-methyl-1-propanol	1.28	0.12	25.64
2-methyl-2-propanol	2.19	0.21	50.05
2-pentanol	1.68	0.19	35.28
2-propanol	1.95	0.16	43.63
3-methyl-1-butanol	1.34	0.15	26.80
4-methyl-2-pentanol	1.39	0.17	27.93
butyl acetate	1.17	0.15	20.87
dibutyl ether	0.58	0.09	10.87

diethyl ether	1.65	0.17	38.03
diisopropyl ether	0.86	0.11	17.20
ethanol	2.08	0.14	48.15
ethyl acetate	1.49	0.15	27.42
methyl acetate	1.51	0.13	27.56
pentyl acetate	1.04	0.15	18.31
propylene carbonate	0.46	0.06	5.50
THF	2.92	0.26	67.18

## 2-octenoic acid C<sub>8</sub>H<sub>14</sub>O<sub>2</sub><sup>22</sup>

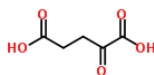


Compound Data			
<b>Molecular weight</b>	142.196	<b>H bond acceptors</b>	2 <b>Rule of 5 violations</b> 0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1 <b>ACD/ALogP</b> 2.93
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	5 <b>Predicted density</b> 0.955 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(O)/C=C/CCCC		
<b>InChIKey</b>	CWMPPVPFLSZGCY-VOTSOKGWSA-N		

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>pp</sub> (g/100g)
methanol	6.64	0.96	11068.64

## 2-oxopentanedioic acid C<sub>5</sub>H<sub>6</sub>O<sub>5</sub><sup>25</sup>

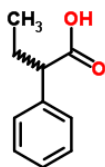


Compound Data			
<b>Molecular weight</b>	146.098	<b>H bond acceptors</b>	5 <b>Rule of 5 violations</b> 0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	2 <b>ACD/ALogP</b> -1.43
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	4 <b>Predicted density</b> 1.499 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(O)C(=O)CCC(=O)O		
<b>InChIKey</b>	KPGXRSRHYNQIFN-UHFFFAOYSA-N		

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>pp</sub> (g/100g)
ethanol	2.99	0.20	79.04
methanol	5.02	0.29	190.70
THF	3.12	0.26	72.46

## 2-phenylbutyric acid C<sub>10</sub>H<sub>12</sub>O<sub>2</sub><sup>79, 83</sup>

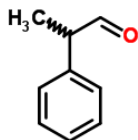


Compound Data			
<b>Molecular weight</b>	164.201	<b>H bond acceptors</b>	2 <b>Rule of 5 violations</b> 0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1 <b>ACD/ALogP</b> 2.38
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	3 <b>Predicted density</b> 1.09 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(O)C(c1ccccc1)CC		
<b>InChIKey</b>	OFJWFNSNDPCAWDK-UHFFFAOYSA-N		

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>pp</sub> (g/100g)
acetonitrile	6.18	0.83	1968.04
DMSO	5.97	0.81	886.12
ethanol	6.2	0.85	1977.18
THF	5.96	0.82	1059.60
toluene	5.35	0.74	519.73

## 2-phenylpropanal C<sub>9</sub>H<sub>10</sub>O<sup>21</sup>



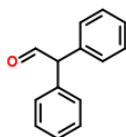
Compound Data			
Molecular weight	134.175	H bond acceptors	1 Rule of 5 violations 0
Compound type	aldehyde	H bond donors	0 ACD/ALogP 2.13
Phase 25°C	liquid	Rotatable bonds	2 Predicted density 0.98 g/cm <sup>3</sup>
SMILES	c1ccccc1C(C)C=O		
InChIKey	IQVAERDLDAZARL-UHFFFAOYSA-N		

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	7.53	□	□

□ Solute is very soluble/miscible, conversion fail.

## 2,2-diphenylacetaldehyde C<sub>14</sub>H<sub>12</sub>O<sup>21</sup>



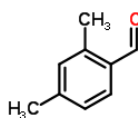
Compound Data			
Molecular weight	196.245	H bond acceptors	1 Rule of 5 violations 0
Compound type	aldehyde	H bond donors	0 ACD/ALogP 3.67
Phase 25°C	liquid	Rotatable bonds	3 Predicted density 1.069 g/cm <sup>3</sup>
SMILES	c1ccccc1C(c1ccccc1)C(=O)		
InChIKey	HLLGFGBLKOIZOM-UHFFFAOYSA-N		

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	5.64	□	□

□ Solute is very soluble/miscible, conversion fail.

## 2,4-dimethylbenzaldehyde C<sub>9</sub>H<sub>10</sub>O<sup>21</sup>

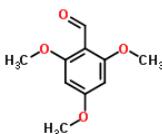


Compound Data			
Molecular weight	134.175	H bond acceptors	1 Rule of 5 violations 0
Compound type	aldehyde	H bond donors	0 ACD/ALogP 2.56
Phase 25°C	liquid	Rotatable bonds	1 Predicted density 1.003 g/cm <sup>3</sup>
SMILES	O=Cc1ccc(C)cc1C		
InChIKey	GISVICWQYMUPJF-UHFFFAOYSA-N		

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	7.17	0.88	3128.10

## 2,4,6-trimethoxybenzaldehyde C<sub>10</sub>H<sub>12</sub>O<sub>4</sub><sup>82</sup>



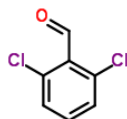
Compound Data			
Molecular weight	196.2	H bond acceptors	4 Rule of 5 violations 0
Compound type	aldehyde	H bond donors	0 ACD/ALogP 1.49
Phase 25°C	solid	Rotatable bonds	4 Predicted density 1.133 g/cm <sup>3</sup>
SMILES	O=Cc1c(OC)cc(OC)cc1OC		
InChIKey	CRBZVDLXAIFERF-UHFFFAOYSA-N		

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
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THF 0.14 0.01 3.11

## 2,6-dichlorobenzaldehyde C<sub>7</sub>H<sub>4</sub>Cl<sub>2</sub>O<sup>208, 205</sup>

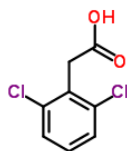


Compound Data					
<b>Molecular weight</b>	175.012	<b>H bond acceptors</b>	1	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	3.03
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	1	<b>Predicted density</b>	1.4 g/cm <sup>3</sup>
<b>SMILES</b>	O=Cc1c(Cl)cccc1Cl				
<b>InChIKey</b>	DMIYKWPEFRFTPY-UHFFFAOYSA-N				

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	1.35	0.08	38.05
chloroform	3.41	0.32	69.35
ethanol	*	*	*
methanol	*	*	*
THF	2.48	0.22	69.58
toluene	1.74	0.19	44.68

\* This aldehyde reacts with alcohols to form a hemiacetal.

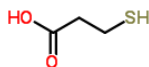
## 2,6-dichlorophenylacetic acid C<sub>8</sub>H<sub>6</sub>Cl<sub>2</sub>O<sub>2</sub><sup>82, 85</sup>



Compound Data					
<b>Molecular weight</b>	205.038	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	2.71
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	2	<b>Predicted density</b>	1.456 g/cm <sup>3</sup>
<b>SMILES</b>	Clc1cccc(Cl)c1CC(=O)O				
<b>InChIKey</b>	SFAILOOQFZNOAU-UHFFFAOYSA-N				

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
THF	3.03	0.30	120.05

## 3-mercaptopropionic acid C<sub>3</sub>H<sub>6</sub>O<sub>2</sub>S<sup>22</sup>



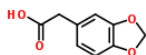
Compound Data					
<b>Molecular weight</b>	106.144	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	0.43
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	3	<b>Predicted density</b>	1.223 g/cm <sup>3</sup>
<b>SMILES</b>	C(CS)C(=O)O				
<b>InChIKey</b>	DKIDEFUBRARXTE-UHFFFAOYSA-N				

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	11.48	0.99	44306.20

## 3,4-(methylenedioxy)phenylacetic acid C<sub>9</sub>H<sub>8</sub>O<sub>4</sub><sup>138</sup>

Compound Data					
<b>Molecular weight</b>	180.157	<b>H bond acceptors</b>	4	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	1.37
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	2	<b>Predicted density</b>	1.406 g/cm <sup>3</sup>



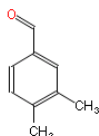


**SMILES** O=C(O)Cc1ccc2OCc2c1  
**InChIKey** ODVLMCWNGKLROU-UHFFFAOYSA-N

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
acetonitrile	0.1	0.01	2.44

### 3,4-dimethylbenzaldehyde C<sub>9</sub>H<sub>10</sub>O<sup>59</sup>



#### Compound Data

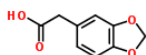
**Molecular weight** 134.175 **H bond acceptors** 1 **Rule of 5 violations** 0  
**Compound type** aldehyde **H bond donors** 0 **ACD/ALogP** 2.56  
**Phase 25°C** liquid **Rotatable bonds** 1 **Predicted density** 1.003 g/cm<sup>3</sup>  
**SMILES** Cc1ccc(cc1C)C=O  
**InChIKey** POQJHLBMLVTHAU-UHFFFAOYSA-N

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
ethanol	7.54	□	□
methanol	7.54	□	□
THF	7.54	□	□

□ Solute is very soluble/miscible, conversion fail.

### 3,4-methylenedioxyphenylacetic acid C<sub>9</sub>H<sub>8</sub>O<sub>4</sub><sup>129, 132, 131</sup>



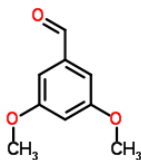
#### Compound Data

**Molecular weight** 180.157 **H bond acceptors** 4 **Rule of 5 violations** 0  
**Compound type** carboxylic acid **H bond donors** 1 **ACD/ALogP** 1.37  
**Phase 25°C** solid **Rotatable bonds** 2 **Predicted density** 1.406 g/cm<sup>3</sup>  
**SMILES** O=C(O)Cc1ccc2OCc2c1  
**InChIKey** ODVLMCWNGKLROU-UHFFFAOYSA-N

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
ethanol	0.55	0.03	13.67
methanol	0.94	0.04	25.57
THF	1.95	0.17	51.81

### 3,5-dimethoxybenzaldehyde C<sub>9</sub>H<sub>10</sub>O<sub>3</sub><sup>205, 208</sup>



#### Compound Data

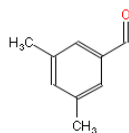
**Molecular weight** 166.174 **H bond acceptors** 3 **Rule of 5 violations** 0  
**Compound type** aldehyde **H bond donors** 0 **ACD/ALogP** 1.53  
**Phase 25°C** solid **Rotatable bonds** 3 **Predicted density** 1.114 g/cm<sup>3</sup>  
**SMILES** O=Cc1cc(OC)cc(OC)c1  
**InChIKey** VFZRZRDOXPRTSC-UHFFFAOYSA-N

#### Solubility Data

Solvent	Concentration	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
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	(M)		
methanol	1.71	0.09	50.66
THF	4.03	0.45	185.73

### 3,5-dimethylbenzaldehyde C<sub>9</sub>H<sub>10</sub>O<sup>63</sup>



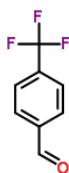
#### Compound Data

<b>Molecular weight</b>	134.175	<b>H bond acceptors</b>	1	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	2.56
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	1	<b>Predicted density</b>	1.003 g/cm <sup>3</sup>
<b>SMILES</b>	Cc1cc(C=O)cc(C)c1				
<b>InChIKey</b>	NBEFMISJJNGCIZ-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
ethanol	7.44	0.99	27092.92
methanol	7.44	0.99	28064.38
THF	7.44	0.99	23376.63

### 4-(trifluoromethyl)benzaldehyde C<sub>8</sub>H<sub>5</sub>F<sub>3</sub>O<sup>21</sup>



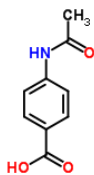
#### Compound Data

<b>Molecular weight</b>	174.12	<b>H bond acceptors</b>	1	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	2.61
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	1	<b>Predicted density</b>	1.293 g/cm <sup>3</sup>
<b>SMILES</b>	c1cc(C=O)ccc1C(F)(F)F				
<b>InChIKey</b>	BEOBZEOPTQQELP-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
methanol	7.32	0.96	11867.65

### 4-acetamidobenzoic acid C<sub>9</sub>H<sub>9</sub>NO<sub>3</sub><sup>137</sup>



#### Compound Data

<b>Molecular weight</b>	179.173	<b>H bond acceptors</b>	4	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	2	<b>ACD/ALogP</b>	1.31
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	2	<b>Predicted density</b>	1.326 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(Nc1ccc(cc1)C(=O)O)C				
<b>InChIKey</b>	QCXJEYYXVJIFCE-UHFFFAOYSA-N				

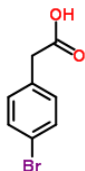
#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
acetonitrile	0.01	0.00	0.24
benzene	0.00	0.00	0.00
ethanol	0.23	0.01	5.45
methanol	0.19	0.01	4.64
THF	0.17	0.01	3.45

### 4-bromophenylacetic acid C<sub>8</sub>H<sub>7</sub>BrO<sub>2</sub><sup>85</sup>

#### Compound Data

<b>Molecular weight</b>	215.044	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
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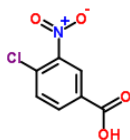


<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	2.28
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	2	<b>Predicted density</b>	1.616 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>Brc1ccc(cc1)CC(=O)O</chem>				
<b>InChIKey</b>	QOWSWEBLNVACCL-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
THF	3.68	0.37	171.85

### 4-chloro-3-nitrobenzoic C<sub>7</sub>H<sub>4</sub>ClNO<sub>4</sub><sup>905</sup>



<b>Molecular weight</b>	201.564	<b>H bond acceptors</b>	5	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	2.37
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	2	<b>Predicted density</b>	1.602 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>O=[N+]([O-])c1cc(ccc1Cl)C(=O)O</chem>				
<b>InChIKey</b>	DFXQXFGFOLXAPO-UHFFFAOYSA-N				

#### Compound Data

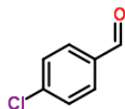
#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
1-butanol	0.31	0.03	8.08
1-decanol	0.19	0.04	4.74
1-heptanol	0.25	0.04	6.34
1-hexanol	0.27	0.03	6.90
1-octanol	0.23	0.04	5.80
1-pentanol	0.27	0.03	6.95
1-propanol	0.37	0.03	9.84
1,4-dioxane	1.43	0.13	35.32
2-butanol	0.32	0.03	8.39
2-ethyl-1-hexanol	0.15	0.02	3.75
2-methyl-1-pentanol	0.19	0.02	4.82
2-methyl-1-propanol	0.19	0.02	4.90
2-methyl-2-propanol	0.38	0.04	10.01
2-pentanol	0.3	0.03	7.77
2-propanol	0.39	0.03	10.45
3-methyl-1-butanol	0.24	0.03	6.17
4-methyl-2-pentanol	0.23	0.03	5.89
butyl acetate	0.23	0.03	5.39
dibutyl ether	0.05	0.01	1.30
diethyl ether	0.24	0.02	6.80
diisopropyl ether	0.1	0.01	2.69
ethanol	0.55	0.03	15.27
ethyl acetate	0.36	0.04	8.46
methyl acetate	0.44	0.04	10.34
methyl butyrate	0.21	0.02	4.88
pentyl acetate	0.16	0.02	3.73
propyl acetate	0.26	0.03	6.08
propylene carbonate	0.15	0.02	2.56
THF	1.95	0.17	57.61

### 4-chlorobenzaldehyde C<sub>7</sub>H<sub>5</sub>ClO<sup>7, 209</sup>

#### Compound Data

<b>Molecular weight</b>	140.567	<b>H bond acceptors</b>	1	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	2.21

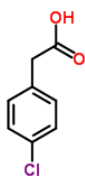


<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	1	<b>Predicted density</b>	1.243 g/cm <sup>3</sup>
<b>SMILES</b>	O=Cc1ccc(Cl)cc1				
<b>InChIKey</b>	AVPYQKSLYISFPO-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	5.59	0.45	285.27
chloroform	3.61	0.33	57.17
ethanol	2.81	0.20	74.23
methanol	3.55	0.20	110.72
THF	5.29	0.51	204.25

### 4-chlorophenylacetic acid C<sub>8</sub>H<sub>7</sub>ClO<sub>2</sub><sup>4, 75, 73</sup>



#### Compound Data

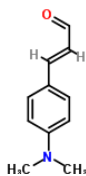
<b>Molecular weight</b>	170.593	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	2.1
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	2	<b>Predicted density</b>	1.324 g/cm <sup>3</sup>
<b>SMILES</b>	Clc1ccc(cc1)CC(=O)O				
<b>InChIKey</b>	CDPKJZJVTHSESZ-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	1.67	0.10	48.72
DMSO	5.74	0.61	342.14
methanol	7.76	□	□
THF	4.45	0.45	197.18
toluene	0.89	0.10	19.69

□ Solute is very soluble/miscible, conversion fail.

### 4-dimethylamino cinnamaldehyde C<sub>11</sub>H<sub>13</sub>NO<sup>3, 32</sup>



#### Compound Data

<b>Molecular weight</b>	175.227	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	2.63
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	3	<b>Predicted density</b>	1.057 g/cm <sup>3</sup>
<b>SMILES</b>	O=CC=Cc1ccc(N(C)C)cc1				
<b>InChIKey</b>	RUKJCCIILMIGEP-ONEGZZNKSA-N				

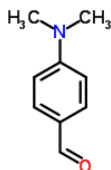
#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.06	0.00	1.25
methanol	0.07	0.00	1.65
THF	0.42	0.03	8.75

### 4-dimethylaminobenzaldehyde C<sub>9</sub>H<sub>11</sub>NO<sup>208, 205</sup>

#### Compound Data

<b>Molecular weight</b>	149.19	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	1.81
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	2	<b>Predicted density</b>	3

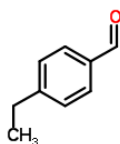


1.072 g/cm

**SMILES** O=Cc1ccc(N(C)C)cc1  
**InChIKey** BGNQWHSBYQYVRX-UHFFFAOYSA-N

**Solubility Data**

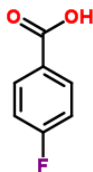
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	2.6	0.18	81.37
chloroform	4.02	0.42	90.76
ethanol	0.63	0.04	13.21
methanol	1.36	0.07	33.24
THF	2.5	0.23	63.27
toluene	1.54	0.17	33.57

**4-ethylbenzaldehyde C<sub>9</sub>H<sub>10</sub>O<sup>63</sup>****Compound Data**

**Molecular weight** 134.175 **H bond acceptors** 1 **Rule of 5 violations** 0  
**Compound type** aldehyde **H bond donors** 0 **ACD/ALogP** 2.63  
**Phase 25°C** liquid **Rotatable bonds** 2 **Predicted density** 1.001 g/cm<sup>3</sup>  
**SMILES** CCc1ccc(C=O)cc1  
**InChIKey** QNGNSVIICDLXHT-UHFFFAOYSA-N

**Solubility Data**

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	7.3	0.95	5840.38
methanol	7.3	0.94	6049.80
THF	7.3	0.96	5039.27

**4-fluorobenzoic acid C<sub>7</sub>H<sub>5</sub>FO<sub>2</sub><sup>106, 121</sup>****Compound Data**

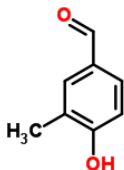
**Molecular weight** 140.112 **H bond acceptors** 2 **Rule of 5 violations** 0  
**Compound type** carboxylic acid **H bond donors** 1 **ACD/ALogP** 2.07  
**Phase 25°C** solid **Rotatable bonds** 1 **Predicted density** 1.319 g/cm<sup>3</sup>  
**SMILES** O=C(O)c1ccc(F)cc1  
**InChIKey** BBYDXOIZLAWGSL-UHFFFAOYSA-N

**Solubility Data**

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.39	0.02	7.63
DMSO	4.19	0.35	96.26
ethanol	0.8	0.05	15.71
methanol	0.76	0.03	15.38
THF	2.49	0.21	52.47
toluene	0.00	0.00	0.00

**4-hydroxy-3-methylbenzaldehyde C<sub>8</sub>H<sub>8</sub>O<sub>2</sub><sup>57</sup>****Compound Data**

**Molecular weight** 136.148 **H bond acceptors** 2 **Rule of 5 violations** 0  
**Compound type** aldehyde **H bond donors** 1 **ACD/ALogP** 1.85

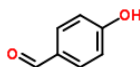


Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.175 g/cm <sup>3</sup>
SMILES	<chem>O=Cc1ccc(O)c(c1)C</chem>				
InChIKey	BAKYASSDAXQKKY-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	2.15	0.14	49.98
methanol	2.78	0.15	74.15
THF	3.05	0.27	71.04

### 4-hydroxybenzaldehyde C<sub>7</sub>H<sub>6</sub>O<sub>2</sub><sup>208, 57, 205, 58, 85, 88</sup>

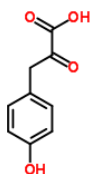


Molecular weight	122.121	H bond acceptors	2	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	1	ACD/ALogP	1.39
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.226 g/cm <sup>3</sup>
SMILES	<chem>O=Cc1ccc(O)cc1</chem>				
InChIKey	RGHHSNMVTDWUBI-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	1.46	0.09	27.93
chloroform	1.75	0.14	17.26
ethanol	2.53	0.17	52.82
methanol	3.4	0.18	83.19
THF	3.7	0.32	79.10
toluene	0.02	0.00	0.28

### 4-hydroxyphenylpyruvic acid C<sub>9</sub>H<sub>8</sub>O<sub>4</sub><sup>15</sup>

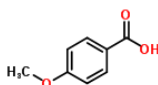


Molecular weight	180.157	H bond acceptors	4	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	2	ACD/ALogP	-0.2
Phase 25°C	solid	Rotatable bonds	4	Predicted density	1.397 g/cm <sup>3</sup>
SMILES	<chem>c1cc(O)ccc1CC(=O)C(=O)O</chem>				
InChIKey	KKADPXVIOXHVK-N-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.71	0.04	18.05
methanol	0.91	0.04	24.67

### 4-methoxybenzoic acid C<sub>8</sub>H<sub>8</sub>O<sub>3</sub><sup>905</sup>

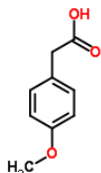


Molecular weight	152.147	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.96
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.207 g/cm <sup>3</sup>
SMILES	<chem>COc1ccc(cc1)C(=O)O</chem>				
InChIKey	ZEYHEAKUIGZSGI-UHFFFAOYSA-N				

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.12	0.01	2.30
1-decanol	0.07	0.01	1.30
1-heptanol	0.09	0.01	1.69
1-hexanol	0.1	0.01	1.89
1-octanol	0.08	0.01	1.49
1-pentanol	0.1	0.01	1.90
1-propanol	0.13	0.01	2.53
1,4-dioxane	0.39	0.04	6.27
2-butanol	0.13	0.01	2.51
2-ethyl-1-hexanol	0.07	0.01	1.31
2-methyl-1-propanol	0.08	0.01	1.54
2-methyl-2-propanol	0.17	0.02	3.29
2-propanol	0.14	0.01	2.74
3-methyl-1-butanol	0.08	0.01	1.52
butyl acetate	0.08	0.01	1.39
dibutyl ether	0.02	0.00	0.39
diethyl ether	0.09	0.01	1.89
diisopropyl ether	0.03	0.00	0.60
ethanol	0.2	0.01	4.00
ethyl acetate	0.13	0.01	2.24
pentyl acetate	0.06	0.01	1.04
THF	0.7	0.06	12.92

### 4-methoxyphenylacetic acid C<sub>9</sub>H<sub>10</sub>O<sub>3</sub><sup>89, 136, 92</sup>



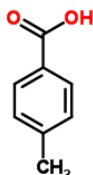
#### Compound Data

Molecular weight	166.174	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.42
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.179 g/cm <sup>3</sup>
SMILES	O=C(O)Cc1ccc(OC)cc1				
InChIKey	NRPFNQDKRYCNX-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	2.23	0.15	72.11
DMSO	4.5	0.47	186.41
methanol	2.5	0.14	85.19
THF	3.32	0.33	114.38
toluene	0.37	0.04	7.45

### 4-methylbenzoic acid C<sub>8</sub>H<sub>8</sub>O<sub>2</sub><sup>2, 25</sup>



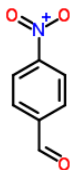
#### Compound Data

Molecular weight	136.148	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.36
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.151 g/cm <sup>3</sup>
SMILES	O=C(O)c1ccc(cc1)C				
InChIKey	LPNBBFKOUUSDB-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.78	0.05	14.89
methanol	0.78	0.04	15.54
THF	1.61	0.14	29.84

## 4-nitrobenzaldehyde C<sub>7</sub>H<sub>5</sub>NO<sub>3</sub><sup>904, 98, 111, 212, 33, 205, 82, 122</sup>



### Compound Data

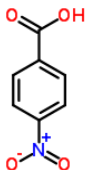
<b>Molecular weight</b>	151.12	<b>H bond acceptors</b>	4	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	1.56
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	2	<b>Predicted density</b>	1.338 g/cm <sup>3</sup>
<b>SMILES</b>	c1cc(C=O)ccc1[N+](=O)[O-]				
<b>InChIKey</b>	BXRFSQSNOROATLV-UHFFFAOYSA-N				

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	*	*	*
1-propanol	*	*	*
2-propanol	*	*	*
acetonitrile	1.13	0.07	26.16
benzene	0.46	0.04	8.40
carbon tetrachloride	0.07	0.01	0.63
chloroform	1.02	0.08	11.57
cyclohexane	0.01	0.00	0.19
dichloromethane	1.29	0.09	18.23
DMF	1.68	0.15	36.02
DMSO	1.24	0.09	19.83
ethanol	*	*	*
ethylene glycol	*	*	*
methanol	*	*	*
THF	0.88	0.07	16.33
toluene	0.46	0.05	8.42

\* This aldehyde reacts with alcohols to form a hemiacetal.

## 4-nitrobenzoic acid C<sub>7</sub>H<sub>5</sub>NO<sub>4</sub><sup>905</sup>



### Compound Data

<b>Molecular weight</b>	167.119	<b>H bond acceptors</b>	5	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	1.89
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	2	<b>Predicted density</b>	1.468 g/cm <sup>3</sup>
<b>SMILES</b>	O=[N+](O-)[C-]1C(=O)OCC1				
<b>InChIKey</b>	OTLNPYWUJOZPPA-UHFFFAOYSA-N				

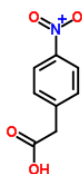
### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.09	0.01	1.89
1-decanol	0.05	0.01	1.01
1-heptanol	0.08	0.01	1.65
1-hexanol	0.08	0.01	1.65
1-octanol	0.06	0.01	1.23
1-pentanol	0.09	0.01	1.87
1-propanol	0.11	0.01	2.34
1,4-dioxane	0.47	0.04	8.34
2-butanol	0.1	0.01	2.11
2-methyl-1-butanol	0.05	0.01	1.04
2-methyl-1-pentanol	0.05	0.01	1.03
2-methyl-1-propanol	0.07	0.01	1.47
2-methyl-2-butanol	0.17	0.02	3.57
2-methyl-2-propanol	0.15	0.01	3.17
2-pentanol	0.08	0.01	1.67
2-propanol	0.11	0.01	2.35



3-methyl-1-butanol	0.07	0.01	1.46
4-methyl-2-pentanol	0.07	0.01	1.45
butyl acetate	0.08	0.01	1.52
dibutyl ether	0.02	0.00	0.43
diethyl ether	0.1	0.01	2.30
diisopropyl ether	0.03	0.00	0.66
ethanol	0.14	0.01	3.05
ethyl acetate	0.13	0.01	2.46
methanol	0.18	0.01	4.08
methyl acetate	0.14	0.01	2.62
pentyl acetate	0.05	0.01	0.95
propylene carbonate	0.06	0.01	0.84
THF	0.78	0.06	15.82

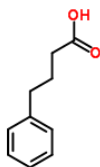
### 4-nitrophenylacetic acid C<sub>8</sub>H<sub>7</sub>NO<sub>4</sub><sup>15</sup>



Compound Data					
<b>Molecular weight</b>	181.145	<b>H bond acceptors</b>	5	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	1.24
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	3	<b>Predicted density</b>	1.407 g/cm <sup>3</sup>
<b>SMILES</b>	c1cc(CC(=O)O)ccc1[N+](=O)[O-]				
<b>InChIKey</b>	YBADLXQNJCMBKR-UHFFFAOYSA-N				

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.71	0.04	18.15
methanol	1.29	0.06	37.21

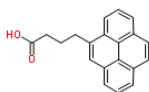
### 4-phenylbutyric acid C<sub>10</sub>H<sub>12</sub>O<sub>2</sub><sup>72</sup>



Compound Data					
<b>Molecular weight</b>	164.201	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	2.42
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	4	<b>Predicted density</b>	1.095 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(O)CCCC1=CC=CC=C1				
<b>InChIKey</b>	OBKXEAXTFZPCHS-UHFFFAOYSA-N				

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-hexanol	0.19	0.02	3.94
chloroform	3.99	0.44	108.74
diethyl ether	4.02	0.51	226.42
methanol	4.54	0.38	310.15
toluene	4.06	0.52	195.66

### 4-pyrenebutanoic acid C<sub>20</sub>H<sub>16</sub>O<sub>2</sub><sup>61, 99, 51, 24, 30, 84, 91</sup>



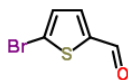
Compound Data					
<b>Molecular weight</b>	288.34	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	1
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	5.37
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	4	<b>Predicted density</b>	1.296 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(O)CCCc4cc2cccc1ccc3c(c12)c4ccc3				
<b>InChIKey</b>	GSBSDUZVSTUKA-UHFFFAOYSA-N				

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
2-propanol	0.06	0.00	2.22
acetonitrile	0.00	0.00	0.00
benzene	0.00	0.00	0.00
carbon tetrachloride	0.00	0.00	0.00
chloroform	0.03	0.00	0.58
cyclohexane	0.00	0.00	0.00
cyclopentane	0.00	0.00	0.00
dichloromethane	0.07	0.00	1.64
diethyl ether	0.02	0.00	0.79
DMF	1.88	0.21	107.11
DMSO	2.07	0.21	100.37
ethanol	0.06	0.00	2.25
hexane	0.00	0.00	0.00
methanol	0.01	0.00	0.51
THF	0.55	0.05	19.99
toluene	0.00	0.00	0.00

### 5-bromothiophene-2-carbaldehyde C<sub>5</sub>H<sub>3</sub>BrOS<sup>21</sup>

#### Compound Data



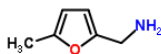
<b>Molecular weight</b>	191.046	<b>H bond acceptors</b>	1	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	1.97
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	1	<b>Predicted density</b>	1.789 g/cm <sup>3</sup>
<b>SMILES</b>	C1=C(SC(=C1)Br)C=O				
<b>InChIKey</b>	GFBVUFQNHLCXPX-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.22	0.96	15186.93

### 5-methylfurfurylamine C<sub>6</sub>H<sub>9</sub>NO<sup>26</sup>

#### Compound Data



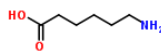
<b>Molecular weight</b>	111.142	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	amine	<b>H bond donors</b>	2	<b>ACD/ALogP</b>	0.71
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	2	<b>Predicted density</b>	1.024 g/cm <sup>3</sup>
<b>SMILES</b>	o1c(ccc1CN)C				
<b>InChIKey</b>	YSEAGSCGERFGBL-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.97	0.94	5010.81

### 6-aminocaproic acid C<sub>6</sub>H<sub>13</sub>NO<sub>2</sub><sup>14</sup>

#### Compound Data

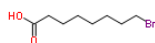


<b>Molecular weight</b>	131.173	<b>H bond acceptors</b>	3	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	3	<b>ACD/ALogP</b>	-0.11
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	6	<b>Predicted density</b>	1.042 g/cm <sup>3</sup>
<b>SMILES</b>	C(CCC(=O)O)CCN				
<b>InChIKey</b>	SLXKOJJOQWFEPD-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.00	0.00	0.00
methanol	0.06	0.00	1.05

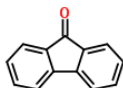
## 8-bromooctanoic acid C<sub>8</sub>H<sub>15</sub>BrO<sub>2</sub><sup>3, 66</sup>



Compound Data				
<b>Molecular weight</b>	223.107	<b>H bond acceptors</b>	2 <b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1 <b>ACD/ALogP</b>	2.76
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	7 <b>Predicted density</b>	1.324 g/cm <sup>3</sup>
<b>SMILES</b>	BrCCCCCCCC(=O)O			
<b>InChIKey</b>	BKJFDZSBZWHRNH-UHFFFAOYSA-N			

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	4.07	0.43	370.56
methanol	3.28	0.24	217.27
THF	3.56	0.42	219.59

## 9-fluorenone C<sub>13</sub>H<sub>8</sub>O<sup>905</sup>

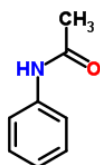


Compound Data				
<b>Molecular weight</b>	180.202	<b>H bond acceptors</b>	1 <b>Rule of 5 violations</b>	0
<b>Compound type</b>	non-Ugi related	<b>H bond donors</b>	0 <b>ACD/ALogP</b>	3.58
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	0 <b>Predicted density</b>	1.244 g/cm <sup>3</sup>
<b>SMILES</b>	O=C3c1ccccc1c2c3ccccc2			
<b>InChIKey</b>	YLQWCDOCJODRMT-UHFFFAOYSA-N			

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.37	0.03	8.75
1-decanol	0.42	0.08	9.73
1-heptanol	0.43	0.06	10.08
1-hexanol	0.41	0.05	9.63
1-octanol	0.43	0.07	10.04
1-pentanol	0.41	0.05	9.69
1-propanol	0.38	0.03	9.12
2-butanol	0.33	0.03	7.80
2-ethyl-1-hexanol	0.35	0.06	8.09
2-methyl-1-pentanol	0.36	0.05	8.41
2-methyl-1-propanol	0.25	0.02	5.84
2-methyl-2-butanol	0.4	0.04	9.43
2-methyl-2-propanol	0.31	0.03	7.27
2-pentanol	0.35	0.04	8.21
2-propanol	0.29	0.02	6.90
2,2,4-trimethylpentane	0.07	0.01	1.80
3-methyl-1-butanol	0.31	0.03	7.23
4-methyl-2-pentanol	0.29	0.04	6.73
acetonitrile	1.57	0.10	49.02
benzene	2.61	0.27	86.63
butyronitrile	1.93	0.19	61.50
carbon tetrachloride	1.83	0.18	26.44
cyclohexane	0.15	0.02	3.50
cyclooctane	0.17	0.02	3.98
cyclopentanol	0.82	0.07	16.70
decane	0.12	0.02	3.00

dibutyl ether	0.37	0.06	9.03
dichloromethane	4.03	0.40	139.36
diethyl ether	0.88	0.09	24.76
diisopropyl ether	0.37	0.05	9.29
ethanol	3.08	0.25	128.48
heptane	0.11	0.02	2.90
hexadecane	0.12	0.03	2.85
hexane	0.1	0.01	2.71
methanol	0.37	0.02	9.36
methyl tert-butyl ether	0.76	0.09	20.52
methylcyclohexane	0.14	0.02	3.32
nonane	0.12	0.02	3.04
octane	0.11	0.02	2.83
propionitrile	1.99	0.17	65.35
tert-butylcyclohexane	0.12	0.02	2.71
toluene	2.17	0.25	65.48
undecane	0.12	0.03	2.96

### acetanilide C<sub>8</sub>H<sub>9</sub>NO<sup>35</sup>



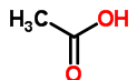
#### Compound Data

<b>Molecular weight</b>	135.163	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	amide	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	1.08
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	1	<b>Predicted density</b>	1.103 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(Nc1ccccc1)C				
<b>InChIKey</b>	FZERHIULMFGESH-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetone	1.42	0.11	30.10

### acetic acid C<sub>2</sub>H<sub>4</sub>O<sub>2</sub><sup>22</sup>



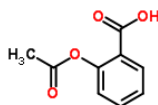
#### Compound Data

<b>Molecular weight</b>	60.052	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	-0.29
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	0	<b>Predicted density</b>	1.068 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(O)C				
<b>InChIKey</b>	QTBSBXVTEAMEQO-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	17.47	0.98	7876.42

### acetylsalicylic acid C<sub>9</sub>H<sub>8</sub>O<sub>4</sub><sup>72, 34, 903</sup>



#### Compound Data

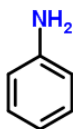
<b>Molecular weight</b>	180.157	<b>H bond acceptors</b>	4	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	1.19
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	3	<b>Predicted density</b>	1.29 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(Oc1ccccc1C(=O)O)C				
<b>InChIKey</b>	BSYNYRMUTXBXSQ-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration	Mole Fraction (X)	pph (g/100g)
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	(M)		
1-hexanol	0.00	0.00	0.00
chloroform	0.18	0.01	2.24
diethyl ether	0.17	0.02	4.27
methanol	1.3	0.06	38.00
toluene	0.00	0.00	0.00

## aniline C<sub>6</sub>H<sub>7</sub>N<sup>29</sup>

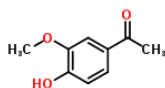


Compound Data			
<b>Molecular weight</b>	93.1265	<b>H bond acceptors</b>	1 <b>Rule of 5 violations</b> 0
<b>Compound type</b>	amine	<b>H bond donors</b>	2 <b>ACD/ALogP</b> 0.94
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	1 <b>Predicted density</b> 1.015 g/cm <sup>3</sup>
<b>SMILES</b>	Nc1ccccc1		
<b>InChIKey</b>	PAYRUJLWNCNPSJ-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	10.97	□	□

□ Solute is very soluble/miscible, conversion fail.

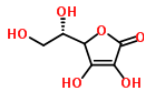
## apocynin C<sub>9</sub>H<sub>10</sub>O<sub>3</sub><sup>906</sup>



Compound Data			
<b>Molecular weight</b>	166.174	<b>H bond acceptors</b>	3 <b>Rule of 5 violations</b> 0
<b>Compound type</b>	non-Ugi related	<b>H bond donors</b>	1 <b>ACD/ALogP</b> 1.39
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	3 <b>Predicted density</b> 1.158 g/cm <sup>3</sup>
<b>SMILES</b>	Oc1ccc(cc1OC)C(C)=O		
<b>InChIKey</b>	DFYRUELUNQRZTB-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-propanol	0.32	0.02	7.01
1,2-dichloroethane	0.41	0.04	6.17
butanone	0.66	0.06	15.41
toluene	0.06	0.01	1.15

## ascorbic acid C<sub>6</sub>H<sub>8</sub>O<sub>6</sub><sup>72</sup>



Compound Data			
<b>Molecular weight</b>	176.124	<b>H bond acceptors</b>	6 <b>Rule of 5 violations</b> 0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	4 <b>ACD/ALogP</b> †
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	6 <b>Predicted density</b> 1.954 g/cm <sup>3</sup>
<b>SMILES</b>	O=C1=C(O)C(=O)O[C@@H]1[C@@H](O)CO		
<b>InChIKey</b>	CIWBShSKHKDKBQ-JLAZNSOCSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-hexanol	0.00	0.00	0.00
chloroform	0.00	0.00	0.00
diethyl ether	0.00	0.00	0.00
toluene	0.00	0.00	0.00

† ACD/ALogP prediction fail.

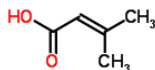
## azoxydibenzoic acid C<sub>14</sub>H<sub>10</sub>N<sub>2</sub>O<sub>5</sub><sup>72</sup>



Compound Data			
<b>Molecular weight</b>	286.24	<b>H bond acceptors</b>	7
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	2
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	4
<b>SMILES</b>	O=C(O)c2ccc([N+](=O)N/c1ccc(cc1)C(=O)O)cc2		
<b>InChIKey</b>	ZYVHVHGJGLOEEKD-NXVVXOECSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	p <sub>pp</sub> (g/100g)
1-hexanol	0.00	0.00	0.00
chloroform	0.00	0.00	0.00
diethyl ether	0.00	0.00	0.00
toluene	0.00	0.00	0.00

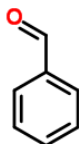
## B,B-dimethylacrylic acid C<sub>5</sub>H<sub>8</sub>O<sub>2</sub><sup>136</sup>



Compound Data			
<b>Molecular weight</b>	100.116	<b>H bond acceptors</b>	2
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	1
<b>SMILES</b>	O=C(O)\C=C(/C)C		
<b>InChIKey</b>	YYPNJNDODFVZLE-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	p <sub>pp</sub> (g/100g)
methanol	4.73	0.27	118.40

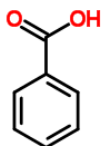
## benzaldehyde C<sub>7</sub>H<sub>6</sub>O<sup>21</sup>



Compound Data			
<b>Molecular weight</b>	106.122	<b>H bond acceptors</b>	1
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	1
<b>SMILES</b>	c1ccccc1C=O		
<b>InChIKey</b>	HUMNYLRZRPPJDN-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	p <sub>pp</sub> (g/100g)
methanol	9.85	0.99	39374.95

## benzoic acid C<sub>7</sub>H<sub>6</sub>O<sub>2</sub><sup>37, 902, 58, 5, 43, 136, 9, 900</sup>

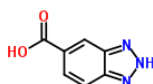


Compound Data			
<b>Molecular weight</b>	122.121	<b>H bond acceptors</b>	2
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	1
<b>SMILES</b>	c1ccccc1C(=O)O		
<b>InChIKey</b>	WPYMKLBDIGXBTP-UHFFFAOYSA-N		

Solubility Data			
Concentration			

Solvent	(M)	Mole Fraction (X)	pph (g/100g)
acetone	1.35	0.11	24.77
acetonitrile	0.76	0.04	13.37
benzene	0.48	0.04	7.06
chloroform	1.8	0.15	17.95
ethanol	2.52	0.17	53.18
methanol	2.84	0.15	64.89
THF	3.37	0.29	69.27
toluene	0.65	0.07	9.81
water	0.03	0.00	0.37

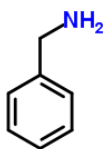
## benzotriazole-5-carboxylic acid $C_7H_5N_3O_2$ <sup>3,32</sup>



Compound Data			
Molecular weight	163.133	H bond acceptors	5 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	2 ACD/ALogP 0.82
Phase 25°C	solid	Rotatable bonds	1 Predicted density 1.617 g/cm <sup>3</sup>
SMILES	O=C(O)c1ccc2nnnc2c1		
InChIKey			

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.04	0.00	0.73
methanol	0.04	0.00	0.76
THF	0.02	0.00	0.36

## benzylamine $C_7H_9N$ <sup>29</sup>

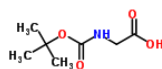


Compound Data			
Molecular weight	107.153	H bond acceptors	1 Rule of 5 violations 0
Compound type	amine	H bond donors	2 ACD/ALogP 1.09
Phase 25°C	liquid	Rotatable bonds	2 Predicted density 0.979 g/cm <sup>3</sup>
SMILES	NCc1ccccc1		
InChIKey	WGQKYBSKWIADBV-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.16	□	□

□ Solute is very soluble/miscible, conversion fail.

## boc-glycine $C_7H_{13}NO_4$ <sup>143, 71, 207, 116, 133, 135</sup>

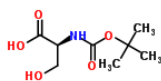


Compound Data			
Molecular weight	175.182	H bond acceptors	5 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	2 ACD/ALogP 0.75
Phase 25°C	solid	Rotatable bonds	4 Predicted density 1.159 g/cm <sup>3</sup>
SMILES	O=C(OC(C)(C)C)NCC(=O)O		
InChIKey	VRPJIFMKZZEXLR-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
2-propanol	3.63	0.38	177.58
acetonitrile	2.46	0.18	91.84
benzene	0.26	0.02	5.32

chloroform	3.85	0.42	107.55
dichloromethane	4.14	0.43	154.79
diethyl ether	2.65	0.31	105.51
DMSO	4.78	0.55	274.57
ethanol	4.11	0.39	243.70
hexane	0.25	0.03	6.74
methanol	4.73	0.41	384.60
THF	3.72	0.40	164.41
toluene	0.19	0.02	3.93

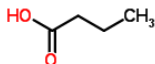
### boc-serine C<sub>8</sub>H<sub>15</sub>NO<sub>5</sub><sup>98, 85</sup>



Compound Data			
Molecular weight	205.208	H bond acceptors	6 Rule of 5 violations 0
Compound type	boc serine	H bond donors	3 ACD/ALogP 0.22
Phase 25°C	solid	Rotatable bonds	6 Predicted density 1.24 g/cm <sup>3</sup>
SMILES	O=C(OC(C)(C)C)N[C@H](C(=O)O)CO		
InChIKey	FHOAKXBXY SJBGX-YFKPBYRVSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
methanol	3.62	0.28	246.06
THF	3.11	0.34	145.78

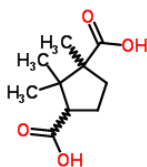
### butyric acid C<sub>4</sub>H<sub>8</sub>O<sub>2</sub><sup>22</sup>



Compound Data			
Molecular weight	88.1051	H bond acceptors	2 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 0.78
Phase 25°C	liquid	Rotatable bonds	2 Predicted density 0.987 g/cm <sup>3</sup>
SMILES	CCCC(=O)O		
InChIKey	FERIUCNNQJTOY-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
methanol	10.94	0.95	5462.12

### camphoric acid C<sub>10</sub>H<sub>16</sub>O<sub>4</sub><sup>902</sup>



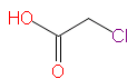
Compound Data			
Molecular weight	200.232	H bond acceptors	4 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	2 ACD/ALogP 1.47
Phase 25°C	solid	Rotatable bonds	2 Predicted density 1.177 g/cm <sup>3</sup>
SMILES	O=C(O)C1CCC(C(=O)O)(C)C1(C)C		
InChIKey	LSPHULWDVZXLIL-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
1-propanol	1.72	0.16	61.24
methanol	2.75	0.18	137.41

### chloroacetic acid C<sub>2</sub>H<sub>3</sub>ClO<sub>2</sub><sup>95</sup>

Compound Data  
32





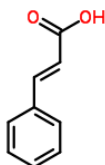
<b>Molecular weight</b>	94.497	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	†
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	1	<b>Predicted density</b>	1.398 g/cm <sup>3</sup>
<b>SMILES</b>	CICC(O)=O				
<b>InChIKey</b>	FOCAUTSVDIKZOP-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	12.45	0.81	993.98
DMSO	11.2	0.77	396.40
methanol	9.45	0.53	328.30
THF	9.63	0.69	288.10
toluene	1.41	0.14	16.95

† ACD/ALogP prediction fail.

### cinnamic acid C<sub>9</sub>H<sub>8</sub>O<sub>2</sub><sup>72, 902, 48</sup>

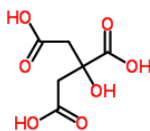


Compound Data					
<b>Molecular weight</b>	148.159	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	2.41
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	2	<b>Predicted density</b>	1.184 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(O)C=Cc1ccccc1				
<b>InChIKey</b>	WBYWAXJHAXSJNI-VOTSOKGWSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-hexanol	0.00	0.00	0.00
chloroform	0.93	0.08	10.40
diethyl ether	0.43	0.04	9.17
ethanol	0.86	0.05	18.31
methanol	1.1	0.05	25.19
toluene	0.3	0.03	5.30

### citric acid anhydrous C<sub>6</sub>H<sub>8</sub>O<sub>7</sub><sup>902, 25</sup>



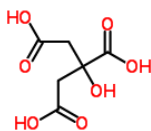
Compound Data					
<b>Molecular weight</b>	192.124	<b>H bond acceptors</b>	7	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	4	<b>ACD/ALogP</b>	-1.72
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	6	<b>Predicted density</b>	1.762 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(O)CC(O)(C(=O)O)CC(=O)O				
<b>InChIKey</b>	KRKNYBCHXYNGOX-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
chloroform	0.00	0.00	0.00
ethanol	1.6	0.10	47.74
methanol	3.08	0.16	118.32
THF	1.8	0.15	47.60

### citric acid monohydrate C<sub>6</sub>H<sub>8</sub>O<sub>7</sub><sup>2</sup>

Compound Data					
<b>Molecular weight</b>	192.124	<b>H bond acceptors</b>	7	<b>Rule of 5 violations</b>	0

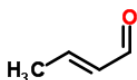


<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	4	<b>ACD/ALogP</b>	-1.72
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	6	<b>Predicted density</b>	1.762 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>O=C(O)CC(O)(C(=O)O)CC(=O)O</chem>				
<b>InChIKey</b>	KRKNYBCHXYNGOX-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
ethanol	1.78	0.12	54.40
methanol	2.27	0.11	76.97
THF	1.52	0.13	38.72

### crotonaldehyde C<sub>4</sub>H<sub>6</sub>O<sup>21</sup>



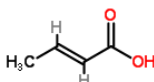
<b>Molecular weight</b>	70.0898	<b>H bond acceptors</b>	1	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	0.51
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	1	<b>Predicted density</b>	0.819 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>CC=CC=O</chem>				
<b>InChIKey</b>	MLUCVPSAIODCQM-NSCUHMNNSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
methanol	12.17	□	□

□ Solute is very soluble/miscible, conversion fail.

### crotonic acid C<sub>4</sub>H<sub>6</sub>O<sub>2</sub><sup>64, 62</sup>



<b>Molecular weight</b>	86.0892	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	0.8
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	1	<b>Predicted density</b>	1.039 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>O=C(O)/C=C/C</chem>				
<b>InChIKey</b>	LDHQZJRKDOVOX-NSCUHMNNSA-N				

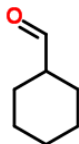
#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
acetonitrile	3.59	0.22	58.89
benzene	4.45	0.39	69.51
chloroform	7.34	0.60	107.51
DMSO	7.76	0.61	170.26
ethanol	6.15	0.43	138.41
hexane	1.07	0.13	14.97
methanol	7.62	0.47	236.33
THF	8.09	0.66	233.69
toluene	3.52	0.34	49.12

### cyclohexanecarbaldehyde C<sub>7</sub>H<sub>12</sub>O<sup>21</sup>

#### Compound Data

<b>Molecular weight</b>	112.17	<b>H bond acceptors</b>	1	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	1.9
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	1	<b>Predicted density</b>	



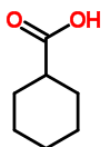
0.992 g/cm

**SMILES** C1CCC(CC1)C=O  
**InChIKey** KVFDZFBHBWTVID-UHFFFAOYSA-N

**Solubility Data**

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
methanol	8.29	0.85	1972.34

**cyclohexanecarboxylic acid C<sub>7</sub>H<sub>12</sub>O<sub>2</sub><sup>22</sup>**



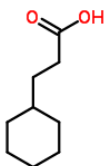
**Compound Data**

**Molecular weight** 128.169    **H bond acceptors** 2    **Rule of 5 violations** 0  
**Compound type** carboxylic acid    **H bond donors** 1    **ACD/ALogP** 1.77  
**Phase 25°C** liquid    **Rotatable bonds** 1    **Predicted density** 1.079 g/cm<sup>3</sup>  
**SMILES** C1CCC(CC1)C(=O)O  
**InChIKey** NZNMSOFKMUBTKW-UHFFFAOYSA-N

**Solubility Data**

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
methanol	8.06	0.89	3220.96

**cyclohexanepropionic acid C<sub>9</sub>H<sub>16</sub>O<sub>2</sub><sup>22</sup>**



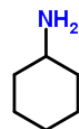
**Compound Data**

**Molecular weight** 156.222    **H bond acceptors** 2    **Rule of 5 violations** 0  
**Compound type** carboxylic acid    **H bond donors** 1    **ACD/ALogP** 2.84  
**Phase 25°C** liquid    **Rotatable bonds** 3    **Predicted density** 1.006 g/cm<sup>3</sup>  
**SMILES** C1CCC(CC1)CCC(=O)O  
**InChIKey** HJZLEGIHUQOJBA-UHFFFAOYSA-N

**Solubility Data**

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
methanol	5.84	0.73	1301.33

**cyclohexylamine C<sub>6</sub>H<sub>13</sub>N<sup>29</sup>**



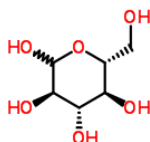
**Compound Data**

**Molecular weight** 99.1741    **H bond acceptors** 1    **Rule of 5 violations** 0  
**Compound type** amine    **H bond donors** 2    **ACD/ALogP** 1.4  
**Phase 25°C** liquid    **Rotatable bonds** 1    **Predicted density** 0.869 g/cm<sup>3</sup>  
**SMILES** NC1CCCCC1  
**InChIKey** PAFZNILMFXMIY-UHFFFAOYSA-N

**Solubility Data**

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
methanol	8.74	0.99	45092.19

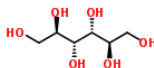
**D-glucose C<sub>6</sub>H<sub>12</sub>O<sub>6</sub><sup>1, 207</sup>**



Compound Data			
Molecular weight	180.156	H bond acceptors	6 Rule of 5 violations 1
Compound type	non-Ugi related	H bond donors	5 ACD/ALogP -1.88
Phase 25°C	solid	Rotatable bonds	6 Predicted density 1.732 g/cm <sup>3</sup>
SMILES	O[C@H]1[C@H](O)[C@H](OC(O)[C@@H]1O)CO		
InChIKey	WQZGKKKJLJFFOK-GASJEMHNSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.01	0.00	0.12
methanol	0.04	0.00	0.84
THF	0.02	0.00	0.30

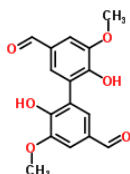
## D-mannitol C<sub>6</sub>H<sub>14</sub>O<sub>6</sub><sup>1,207</sup>



Compound Data			
Molecular weight	182.172	H bond acceptors	6 Rule of 5 violations 1
Compound type	non-Ugi related	H bond donors	6 ACD/ALogP -4.67
Phase 25°C	solid	Rotatable bonds	11 Predicted density 1.596 g/cm <sup>3</sup>
SMILES	O[C@H]([C@H](O)CO)[C@H](O)[C@H](O)CO		
InChIKey	FBPFZTCFMRRESA-KVTDHHQDSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.01	0.00	0.12
methanol	0.01	0.00	0.24
THF	0.02	0.00	0.30

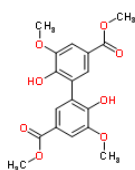
## dehydrodivanillin C<sub>16</sub>H<sub>14</sub>O<sub>6</sub><sup>906</sup>



Compound Data			
Molecular weight	302.279	H bond acceptors	6 Rule of 5 violations 0
Compound type	non-Ugi related	H bond donors	2 ACD/ALogP 1.57
Phase 25°C	solid	Rotatable bonds	7 Predicted density 1.356 g/cm <sup>3</sup>
SMILES	O=Cc2cc(c1cc(cc(OC)c1O)C=O)c(O)c(OC)c2		
InChIKey	NSTQUZVZBUTVPY-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-propanol	0.00	0.00	0.00
1,2-dichloroethane	0.00	0.00	0.00
butanone	0.00	0.00	0.00
toluene	0.00	0.00	0.00

## di(methyl vanillate) C<sub>18</sub>H<sub>18</sub>O<sub>8</sub><sup>906</sup>

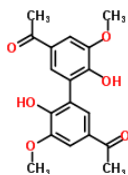


Compound Data			
Molecular weight	362.331	H bond acceptors	8 Rule of 5 violations 0
Compound type	non-Ugi related	H bond donors	2 ACD/ALogP 2.27
Phase 25°C	solid	Rotatable bonds	9 Predicted density 1.315 g/cm <sup>3</sup>
SMILES	O=C(OC)c2cc(c1cc(cc(OC)c1O)C(=O)OC)c(O)c(OC)c2		
InChIKey	DBUKZZKLTUXIQM-UHFFFAOYSA-N		

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-propanol	0.00	0.00	0.00
1,2-dichloroethane	0.01	0.00	0.31
butanone	0.00	0.00	0.00
toluene	0.00	0.00	0.00

### diapocynin C<sub>18</sub>H<sub>18</sub>O<sub>6</sub><sup>906</sup>



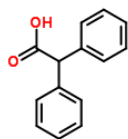
### Compound Data

<b>Molecular weight</b>	330.332	<b>H bond acceptors</b>	6	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	non-Ugi related	<b>H bond donors</b>	2	<b>ACD/ALogP</b>	1.97
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	7	<b>Predicted density</b>	1.257 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(c2cc(c1cc(cc(OC)c1O)C(=O)C)c(O)c(OC)c2)C				
<b>InChIKey</b>	HLNDPICGHQGSU-UHFFFAOYSA-N				

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-propanol	0.00	0.00	0.00
1,2-dichloroethane	0.00	0.00	0.00
butanone	0.00	0.00	0.00
toluene	0.00	0.00	0.00

### diphenylacetic acid C<sub>14</sub>H<sub>12</sub>O<sub>2</sub><sup>81, 77</sup>



### Compound Data

<b>Molecular weight</b>	212.244	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	3.25
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	3	<b>Predicted density</b>	1.174 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(O)C(c1ccccc1)c2ccccc2				
<b>InChIKey</b>	PYHXGXCGESYPCW-UHFFFAOYSA-N				

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.46	0.03	14.26
DMSO	2.56	0.25	92.04
ethanol	1.15	0.08	39.51
methanol	1.27	0.07	46.47
THF	2.91	0.33	144.17
toluene	0.17	0.02	4.27

### formic acid CH<sub>2</sub>O<sub>2</sub><sup>22</sup>



### Compound Data

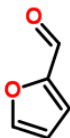
<b>Molecular weight</b>	46.0254	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	-0.54
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	0	<b>Predicted density</b>	1.154 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(O)				
<b>InChIKey</b>	BDAGIHXXWSANSR-UHFFFAOYSA-N				

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	26.5	□	□

□ Solute is very soluble/miscible, conversion fail.

## furfuraldehyde C<sub>5</sub>H<sub>4</sub>O<sub>2</sub><sup>20</sup>



### Compound Data

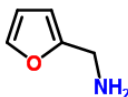
<b>Molecular weight</b>	96.0841	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	0.73
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	1	<b>Predicted density</b>	1.145 g/cm <sup>3</sup>
<b>SMILES</b>	O=Cc1ccco1				
<b>InChIKey</b>	HYBBIBNJHNGZAN-UHFFFAOYSA-N				

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	12.02	□	□

□ Solute is very soluble/miscible, conversion fail.

## furfurylamine C<sub>5</sub>H<sub>7</sub>NO<sup>26</sup>



### Compound Data

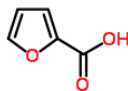
<b>Molecular weight</b>	97.1152	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	amine	<b>H bond donors</b>	2	<b>ACD/ALogP</b>	0.25
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	2	<b>Predicted density</b>	1.053 g/cm <sup>3</sup>
<b>SMILES</b>	o1c(ccc1)CN				
<b>InChIKey</b>	DDRPCXLAQZKBJP-UHFFFAOYSA-N				

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	11.32	□	□

□ Solute is very soluble/miscible, conversion fail.

## furoic acid C<sub>5</sub>H<sub>4</sub>O<sub>3</sub><sup>104</sup>



### Compound Data

<b>Molecular weight</b>	112.084	<b>H bond acceptors</b>	3	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	0.64
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	1	<b>Predicted density</b>	1.322 g/cm <sup>3</sup>
<b>SMILES</b>	OC(=O)c1ccco1				
<b>InChIKey</b>	SMNDYUVBFMFKNZ-UHFFFAOYSA-N				

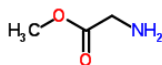
### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	1.1	0.06	18.14
DMSO	6.64	0.52	154.95
methanol	4.12	0.21	94.36
THF	4.07	0.33	77.05
toluene	0.06	0.01	0.78

## glycine methyl ester C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub><sup>207</sup>

### Compound Data

<b>Molecular weight</b>	89.0932	<b>H bond acceptors</b>	3	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	amine	<b>H bond donors</b>	2	<b>ACD/ALogP</b>	-0.83
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	3	<b>Predicted density</b>	1.045 g/cm <sup>3</sup>

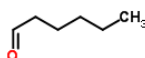


**SMILES** O=C(OC)CN  
**InChIKey** KQSSATDQUYCRGS-UHFFFAOYSA-N

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
ethanol	0.19	0.01	2.21
methanol	1.32	0.06	17.60
THF	0.04	0.00	0.40

### hexanaldehyde C<sub>6</sub>H<sub>12</sub>O<sup>21</sup>



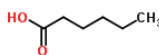
**Compound Data**  
**Molecular weight** 100.159 **H bond acceptors** 1 **Rule of 5 violations** 0  
**Compound type** aldehyde **H bond donors** 0 **ACD/ALogP** 1.97  
**Phase 25°C** liquid **Rotatable bonds** 4 **Predicted density** 0.801 g/cm<sup>3</sup>  
**SMILES** CCCCC=O  
**InChIKey** JARKCYVAAOWBJS-UHFFFAOYSA-N

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
methanol	8.33	□	□

□ Solute is very soluble/miscible, conversion fail.

### hexanoic acid C<sub>6</sub>H<sub>12</sub>O<sub>2</sub><sup>22</sup>

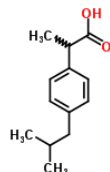


**Compound Data**  
**Molecular weight** 116.158 **H bond acceptors** 2 **Rule of 5 violations** 0  
**Compound type** carboxylic acid **H bond donors** 1 **ACD/ALogP** 1.84  
**Phase 25°C** liquid **Rotatable bonds** 4 **Predicted density** 0.95 g/cm<sup>3</sup>  
**SMILES** CCCCC(=O)O  
**InChIKey** FUZZWVXGSPDMH-UHFFFAOYSA-N

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
methanol	7.98	0.93	5071.51

### ibuprofen C<sub>13</sub>H<sub>18</sub>O<sub>2</sub><sup>905</sup>



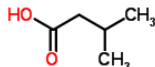
**Compound Data**  
**Molecular weight** 206.281 **H bond acceptors** 2 **Rule of 5 violations** 0  
**Compound type** carboxylic acid **H bond donors** 1 **ACD/ALogP** 3.72  
**Phase 25°C** solid **Rotatable bonds** 4 **Predicted density** 1.029 g/cm<sup>3</sup>  
**SMILES** O=C(O)C(c1ccc(cc1)CC(C)C)C  
**InChIKey** HEFNNWSXXWATRW-UHFFFAOYSA-N

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
1-decanol	1.12	0.22	35.98

1-octanol	1.2	0.20	39.60
1-pentanol	1.46	0.18	52.50
1-propanol	1.52	0.14	56.72
2-butanol	1.78	0.20	71.27
2-methyl-1-propanol	1.76	0.20	70.04
2-propanol	2.22	0.23	104.32
ethanol	1.18	0.08	40.88
methanol	1.16	0.06	41.41

### isovaleric acid C<sub>5</sub>H<sub>10</sub>O<sub>2</sub><sup>22</sup>

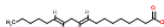


Compound Data					
<b>Molecular weight</b>	102.132	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	1.13
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	2	<b>Predicted density</b>	0.962 g/cm <sup>3</sup>
<b>SMILES</b>	CC(C)CC(=O)O				
<b>InChIKey</b>	GWYFCOCPABKNJV-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.06	0.91	3222.50

### linoleic acid C<sub>18</sub>H<sub>32</sub>O<sub>2</sub><sup>22</sup>

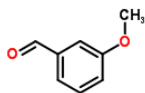


Compound Data					
<b>Molecular weight</b>	280.445	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	1
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	7.18
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	14	<b>Predicted density</b>	0.911 g/cm <sup>3</sup>
<b>SMILES</b>	CCCCC=CCC=CCCCCCCC(=O)O				
<b>InChIKey</b>	OYHQOLUKZRVURQ-AVQMFATSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	3.22	0.94	13712.82

### m-anisaldehyde C<sub>8</sub>H<sub>8</sub>O<sub>2</sub><sup>21</sup>



Compound Data					
<b>Molecular weight</b>	136.148	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	1.65
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	2	<b>Predicted density</b>	1.088 g/cm <sup>3</sup>
<b>SMILES</b>	COc1cc(C=O)ccc1				
<b>InChIKey</b>	WMPDAIZRQDCGFH-UHFFFAOYSA-N				

#### Solubility Data

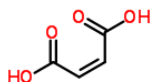
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.2	□	□

□ Solute is very soluble/miscible, conversion fail.

### maleic acid C<sub>4</sub>H<sub>4</sub>O<sub>4</sub><sup>39, 40</sup>

Compound Data					
<b>Molecular weight</b>	116.072	<b>H bond acceptors</b>	4	<b>Rule of 5 violations</b>	0



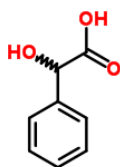


<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	2	<b>ACD/ALogP</b>	-0.01
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	2	<b>Predicted density</b>	1.499 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>C(=C(O)O)C(=O)O</chem>				
<b>InChIKey</b>	VZCYOOQTPOCHFL-OWOJBTEDSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	3.41	0.21	68.95
methanol	3.82	0.19	83.62

### mandelic acid C<sub>8</sub>H<sub>8</sub>O<sub>3</sub><sup>72, 71</sup>

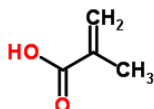


<b>Molecular weight</b>	152.147	<b>H bond acceptors</b>	3	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	2	<b>ACD/ALogP</b>	0.92
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	3	<b>Predicted density</b>	1.321 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>O=C(O)C(O)c1ccccc1</chem>				
<b>InChIKey</b>	IWYDHOAUDWTVEP-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-hexanol	0.00	0.00	0.00
chloroform	0.12	0.01	1.23
diethyl ether	0.77	0.08	17.51
methanol	3.54	0.20	120.77
toluene	0.00	0.00	0.00

### methacrylic acid C<sub>4</sub>H<sub>6</sub>O<sub>2</sub><sup>22</sup>

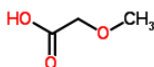


<b>Molecular weight</b>	86.0892	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	0.83
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	1	<b>Predicted density</b>	1.023 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>CC(=C)C(=O)O</chem>				
<b>InChIKey</b>	CERQOIWHTDAKMF-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	11.79	0.98	17218.73

### methoxyacetic acid C<sub>3</sub>H<sub>6</sub>O<sub>3</sub><sup>22</sup>



<b>Molecular weight</b>	90.0779	<b>H bond acceptors</b>	3	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	-0.96
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	2	<b>Predicted density</b>	1.139 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>COCC(=O)O</chem>				
<b>InChIKey</b>	RMIODHQZRUFFFF-UHFFFAOYSA-N				

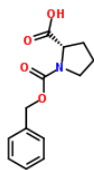
#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
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methanol 13.03 □ □

□ Solute is very soluble/miscible, conversion fail.

### N-Cbz-L-p roline C<sub>13</sub>H<sub>15</sub>NO<sub>4</sub><sup>134</sup>

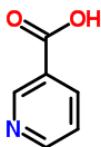


Compound Data			
<b>Molecular weight</b>	249.262	<b>H bond acceptors</b>	5 <b>Rule of 5 violations</b> 0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1 <b>ACD/ALogP</b> 1.17
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	4 <b>Predicted density</b> 1.309 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(O)[C@H]2N(C(=O)OCc1ccccc1)CCC2		
<b>InChIKey</b>	JXGVXCZADZNAMJ-NSHDSACASA-N		

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	4.26	0.49	746.90

### nicotinic acid C<sub>6</sub>H<sub>5</sub>NO<sub>2</sub><sup>100, 137</sup>

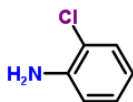


Compound Data			
<b>Molecular weight</b>	123.109	<b>H bond acceptors</b>	3 <b>Rule of 5 violations</b> 0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1 <b>ACD/ALogP</b> 0.15
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	1 <b>Predicted density</b> 1.293 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(O)c1ccnc1		
<b>InChIKey</b>	PVNIIMVLHYAWGP-UHFFFAOYSA-N		

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.00	0.00	0.00
benzene	0.00	0.00	0.00
DMSO	0.57	0.04	6.71
ethanol	0.09	0.01	1.43
methanol	0.06	0.00	1.03
THF	0.06	0.00	0.75
toluene	0.00	0.00	0.00

### o-chloroaniline C<sub>6</sub>H<sub>6</sub>ClN<sup>29</sup>



Compound Data			
<b>Molecular weight</b>	127.572	<b>H bond acceptors</b>	1 <b>Rule of 5 violations</b> 0
<b>Compound type</b>	amine	<b>H bond donors</b>	2 <b>ACD/ALogP</b> 1.91
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	1 <b>Predicted density</b> 1.23 g/cm <sup>3</sup>
<b>SMILES</b>	Nc1ccccc1Cl		
<b>InChIKey</b>	AKCROHQJQJBRMN-UHFFFAOYSA-N		

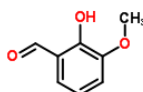
#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.51	0.97	11802.88

### o-vanillin C<sub>8</sub>H<sub>8</sub>O<sub>3</sub><sup>208, 205</sup>

#### Compound Data

<b>Molecular weight</b>	152.147	<b>H bond acceptors</b>	3 <b>Rule of 5 violations</b> 0
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	1 <b>ACD/ALogP</b> 1.4

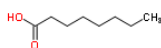


Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.231 g/cm <sup>3</sup>
SMILES	<chem>Oc1c(cccc1OC)C=O</chem>				
InChIKey	JJVNINGBHGBWJH-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
acetonitrile	2.56	0.17	76.28
ethanol	3.04	0.22	94.99
methanol	2.27	0.12	63.75
THF	5.37	0.56	268.76
toluene	3.82	0.43	126.41

### octanoic acid C<sub>8</sub>H<sub>16</sub>O<sub>2</sub><sup>22</sup>



Molecular weight	144.211	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.9
Phase 25°C	liquid	Rotatable bonds	6	Predicted density	0.929 g/cm <sup>3</sup>
SMILES	<chem>CCCCCCCC(=O)O</chem>				
InChIKey	WWZKQHOCKIZLMA-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
methanol	6.31	0.93	5899.86

### octylamine C<sub>8</sub>H<sub>19</sub>N<sup>29</sup>

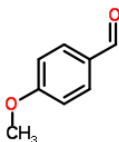


Molecular weight	129.243	H bond acceptors	1	Rule of 5 violations	0
Compound type	amine	H bond donors	2	ACD/ALogP	3.06
Phase 25°C	liquid	Rotatable bonds	7	Predicted density	0.786 g/cm <sup>3</sup>
SMILES	<chem>NCCCCCCCC</chem>				
InChIKey	IOQPZZOEVZRBK-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
methanol	6.05	0.98	20005.33

### p-anisaldehyde C<sub>8</sub>H<sub>8</sub>O<sub>2</sub><sup>21</sup>



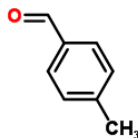
Molecular weight	136.148	H bond acceptors	2	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.7
Phase 25°C	liquid	Rotatable bonds	2	Predicted density	1.088 g/cm <sup>3</sup>
SMILES	<chem>COc1ccc(C=O)cc1</chem>				
InChIKey	ZRSNZINYAWTAHE-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
methanol	8.22	□	□

□ Solute is very soluble/miscible, conversion fail.

## p-tolualdehyde C<sub>8</sub>H<sub>8</sub>O<sup>21</sup>

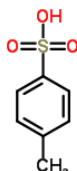


Compound Data			
Molecular weight	120.148	H bond acceptors	1 Rule of 5 violations 0
Compound type	aldehyde	H bond donors	0 ACD/ALogP 2.1
Phase 25°C	liquid	Rotatable bonds	1 Predicted density 1.023 g/cm <sup>3</sup>
SMILES	O=Cc1ccc(C)cc1		
InChIKey	FXLOVSHXALFLKQ-UHFFFAOYSA-N		

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
methanol	8.47	0.99	25859.25

## p-toluenesulfonic acid C<sub>7</sub>H<sub>8</sub>O<sub>3</sub>S<sup>107, 136</sup>

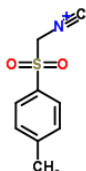


Compound Data			
Molecular weight	172.202	H bond acceptors	3 Rule of 5 violations 0
Compound type	non-Ugi related	H bond donors	1 ACD/ALogP 0.93
Phase 25°C	solid	Rotatable bonds	1 Predicted density 1.34 g/cm <sup>3</sup>
SMILES	O=S(=O)(O)c1ccc(cc1)C		
InChIKey	JOXIMZWYDAKGHI-UHFFFAOYSA-N		

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
acetonitrile	0.12	0.01	2.69
ethanol	4.69	0.41	260.62
toluene	0.00	0.00	0.00

## p-toluenesulfonylmethyl isocyanide C<sub>9</sub>H<sub>9</sub>NO<sub>2</sub>S<sup>208</sup>



Compound Data			
Molecular weight	195.238	H bond acceptors	3 Rule of 5 violations 0
Compound type	isonitrile	H bond donors	0 ACD/ALogP †
Phase 25°C	solid	Rotatable bonds	2 Predicted density ‡
SMILES	O=S(=O)(c1ccc(cc1)C)C[N+]#[C-]		
InChIKey	CFOAUYCPAUGDFF-UHFFFAOYSA-N		

### Solubility Data

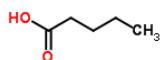
Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
acetonitrile	1.88	‡	‡
chloroform	0.21	‡	‡
ethanol	0.18	‡	‡
THF	1.86	‡	‡
toluene	0.14	‡	‡

† ACD/ALogP prediction fail.

‡ Solute density prediction fail.

## pentanoic acid C<sub>5</sub>H<sub>10</sub>O<sub>2</sub><sup>22</sup>

Compound Data			
Molecular weight	102.132	H bond acceptors	2 Rule of 5 violations 0

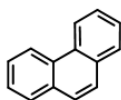


<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	1.31
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	3	<b>Predicted density</b>	0.966 g/cm <sup>3</sup>
<b>SMILES</b>	CCCCC(=O)O				
<b>InChIKey</b>	NQPDZGIKBAWPEJ-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
methanol	9.19	0.93	4393.39

### phenanthrene C<sub>14</sub>H<sub>10</sub><sup>902</sup>

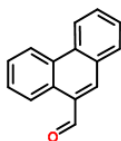


<b>Molecular weight</b>	178.229	<b>H bond acceptors</b>	0	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	non-Ugi related	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	4.68
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	0	<b>Predicted density</b>	1.13 g/cm <sup>3</sup>
<b>SMILES</b>	c3cc2ccc1ccccc1c2cc3				
<b>InChIKey</b>	YNPNZTXNASCQKK-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
benzene	2.02	0.21	60.52
carbon disulfide	3.05	0.26	83.20
carbon tetrachloride	1.73	0.18	24.99
diethyl ether	1.36	0.15	42.04
ethanol	0.21	0.01	4.96
hexane	0.32	0.04	8.90

### phenanthrene-9-carboxaldehyde C<sub>15</sub>H<sub>10</sub>O<sup>30, 60, 4, 136, 242, 51, 24</sup>



<b>Molecular weight</b>	206.239	<b>H bond acceptors</b>	1	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	4.1
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	1	<b>Predicted density</b>	1.217 g/cm <sup>3</sup>
<b>SMILES</b>	O=Cc2cc3c(c1c2ccccc1)ccccc3				
<b>InChIKey</b>	QECIGMPORCORE-UHFFFAOYSA-N				

#### Solubility Data

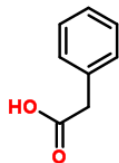
Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
1,1,2-trichlorotrifluoroethane	0.02	0.00	0.25
2-propanol	0.07	0.01	1.85
acetonitrile	0.16	0.01	4.39
benzene	0.66	0.06	17.56
chloroform	0.04	0.00	0.55
cyclohexane	0.07	0.01	1.85
cyclopentane	0.03	0.00	0.79
dichloromethane	0.00	0.00	0.00
diethyl ether	0.1	0.01	2.86
DMF	1.25	0.12	37.60
DMSO	0.77	0.06	16.62
ethanol	0.1	0.01	2.69
hexane	0.07	0.01	2.16
methanol	0.11	0.00	2.93
THF	2.32	0.23	87.22

toluene

0.14

0.01

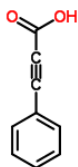
3.40

**phenylacetic acid** C<sub>8</sub>H<sub>8</sub>O<sub>2</sub><sup>86, 123</sup>

Compound Data			
<b>Molecular weight</b>	136.148	<b>H bond acceptors</b>	2 <b>Rule of 5 violations</b> 0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1 <b>ACD/ALogP</b> 1.51
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	2 <b>Predicted density</b> 1.164 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(O)Cc1ccccc1		
<b>InChIKey</b>	WLJVXDMOQOGPHL-UHFFFAOYSA-N		

**Solubility Data**

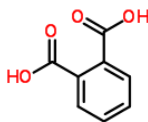
Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
acetonitrile	3.87	0.28	128.87
benzene	3.35	0.33	85.91
DMF	3.76	0.36	105.03
DMSO	6.35	0.64	305.77
THF	5.62	0.57	247.02
toluene	1.94	0.21	39.23

**phenylpropynoic acid** C<sub>9</sub>H<sub>6</sub>O<sub>2</sub><sup>98, 82, 85</sup>

Compound Data			
<b>Molecular weight</b>	146.143	<b>H bond acceptors</b>	2 <b>Rule of 5 violations</b> 0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1 <b>ACD/ALogP</b> 2.61
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	1 <b>Predicted density</b> 1.24 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(C#Cc1ccccc1)O		
<b>InChIKey</b>	XNERWVPQCYSMLC-UHFFFAOYSA-N		

**Solubility Data**

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
acetonitrile	1.38	0.08	32.24
DMSO	3.33	0.28	72.89
methanol	2.89	0.16	85.06
THF	4.34	0.42	143.85

**phthalic acid** C<sub>8</sub>H<sub>6</sub>O<sub>4</sub><sup>138, 47</sup>

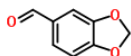
Compound Data			
<b>Molecular weight</b>	166.131	<b>H bond acceptors</b>	4 <b>Rule of 5 violations</b> 0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	2 <b>ACD/ALogP</b> 0.81
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	2 <b>Predicted density</b> 1.451 g/cm <sup>3</sup>
<b>SMILES</b>	O=C(O)c1ccccc1C(=O)O		
<b>InChIKey</b>	XNGIFLGASWRNHJ-UHFFFAOYSA-N		

**Solubility Data**

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
chloroform	0.51	0.04	6.00
methanol	0.43	0.02	9.98

**piperonal** C<sub>8</sub>H<sub>6</sub>O<sub>3</sub><sup>71, 30</sup>**Compound Data**

<b>Molecular weight</b>	150.131	<b>H bond acceptors</b>	3 <b>Rule of 5 violations</b> 0
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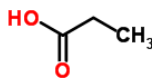


<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	1.05
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	1	<b>Predicted density</b>	1.337 g/cm <sup>3</sup>
<b>SMILES</b>	O=Cc1ccc2OCOCc2c1				
<b>InChIKey</b>	SATCULPHIDQDRE-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	7.11	0.66	708.73
chloroform	7.95	0.86	741.57
dichloromethane	7.59	0.78	616.11
diethyl ether	6.38	0.69	460.15
DMSO	6.05	0.57	257.75
ethanol	4.99	0.40	218.45
hexane	0.15	0.02	3.39
methanol	7.29	0.63	798.18
THF	7.44	0.78	750.82
toluene	6.4	0.71	392.09

### propanoic acid C<sub>3</sub>H<sub>6</sub>O<sub>2</sub><sup>22</sup>

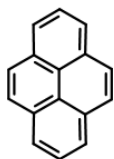


<b>Molecular weight</b>	74.0785	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	0.25
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	1	<b>Predicted density</b>	1.019 g/cm <sup>3</sup>
<b>SMILES</b>	CCC(=O)O				
<b>InChIKey</b>	XBDQKXXYIPTUBI-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	13.41	0.96	5249.72

### pyrene C<sub>16</sub>H<sub>10</sub><sup>108, 109</sup>



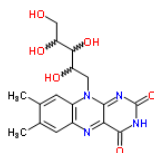
<b>Molecular weight</b>	202.251	<b>H bond acceptors</b>	0	<b>Rule of 5 violations</b>	1
<b>Compound type</b>	non-Ugi related	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	5.17
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	0	<b>Predicted density</b>	1.248 g/cm <sup>3</sup>
<b>SMILES</b>	c3ccc2ccc1cccc4c1c2c3cc4				
<b>InChIKey</b>	BBEAQIROQSPTKN-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.1	0.01	2.75

### riboflavin C<sub>17</sub>H<sub>20</sub>N<sub>4</sub>O<sub>6</sub><sup>46</sup>

<b>Molecular weight</b>	376.364	<b>H bond acceptors</b>	10	<b>Rule of 5 violations</b>	2
<b>Compound type</b>	non-Ugi related	<b>H bond donors</b>	5	<b>ACD/ALogP</b>	-2.02
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	9	<b>Predicted density</b>	1.65 g/cm <sup>3</sup>
<b>SMILES</b>	O=C2N=C1N(c3cc(c(cc3/N=C/1C(=O)N2)C)C)C(O)C(O)C(O)C(O)C				

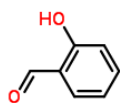


**InChIKey** AUNGANRZJHBGPY-UHFFFAOYSA-N

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.00	0.00	0.00

### salicylaldehyde C<sub>7</sub>H<sub>6</sub>O<sub>2</sub><sup>21</sup>



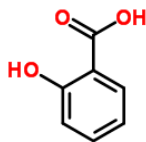
Compound Data			
<b>Molecular weight</b>	122.121	<b>H bond acceptors</b>	2
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	1
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	2
<b>SMILES</b>	c1cccc(C=O)c1O		
<b>InChIKey</b>	SMQUZDBALVYZAC-UHFFFAOYSA-N		

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	10.04	□	□

□ Solute is very soluble/miscible, conversion fail.

### salicylic acid C<sub>7</sub>H<sub>6</sub>O<sub>3</sub><sup>34, 901, 902, 138, 52</sup>

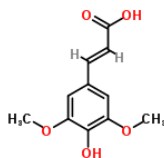


Compound Data			
<b>Molecular weight</b>	138.121	<b>H bond acceptors</b>	3
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	2
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	2
<b>SMILES</b>	O=C(O)c1ccccc1O		
<b>InChIKey</b>	YGSDEFSMJLZEOE-UHFFFAOYSA-N		

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
chloroform	0.19	0.01	1.74
dichloromethane	0.15	0.01	1.68
ethanol	2.34	0.15	54.17
methanol	2.65	0.13	66.24
toluene	0.11	0.01	1.76

### sinapic acid C<sub>11</sub>H<sub>12</sub>O<sub>5</sub><sup>25, 2</sup>



Compound Data			
<b>Molecular weight</b>	224.21	<b>H bond acceptors</b>	5
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	2
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	5
<b>SMILES</b>	O=C(O)C=Cc1cc(OC)c(O)c(OC)c1		
<b>InChIKey</b>	PCMORTLOPMLFEB-ONEGZZNKSAN		

#### Solubility Data

Solvent	Concentration	Mole Fraction (X)	pph (g/100g)
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	(M)		
ethanol	0.79	0.05	26.27
methanol	1.04	0.05	37.69
THF	0.45	0.04	11.95

## sodium chloride $\text{ClNa}^1, 207, 900$



### Compound Data

<b>Molecular weight</b>	58.4428	<b>H bond acceptors</b>	0	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	non-Ugi related	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	†
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	0	<b>Predicted density</b>	‡
<b>SMILES</b>	Cl[Na]				
<b>InChIKey</b>	FAPWRFPFISZLT-UHFFFAOYSA-M				

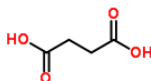
### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.00	0.00	0.00
methanol	0.22	‡	‡
THF	0.04	‡	‡

† ACD/ALogP prediction fail.

‡ Solute density prediction fail.

## succinic acid $\text{C}_4\text{H}_6\text{O}_4^{45, 42, 44}$



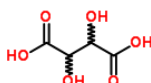
### Compound Data

<b>Molecular weight</b>	118.088	<b>H bond acceptors</b>	4	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	2	<b>ACD/ALogP</b>	-0.59
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	3	<b>Predicted density</b>	1.408 g/cm <sup>3</sup>
<b>SMILES</b>	OC(CCC(O)=O)=O				
<b>InChIKey</b>	KDYFGRWQOYBRFD-UHFFFAOYSA-N				

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
2-propanol	0.34	0.03	5.22
ethanol	0.57	0.03	9.06

## tartaric acid $\text{C}_4\text{H}_6\text{O}_6^{38}$



### Compound Data

<b>Molecular weight</b>	150.087	<b>H bond acceptors</b>	6	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	4	<b>ACD/ALogP</b>	-1.43
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	5	<b>Predicted density</b>	1.886 g/cm <sup>3</sup>
<b>SMILES</b>	C(C(C(=O)O)O)(C(=O)O)O				
<b>InChIKey</b>	FEWJPZIEWOKRBE-UHFFFAOYSA-N				

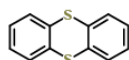
### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetone	0.79	0.06	16.39

## thianthrene $\text{C}_{12}\text{H}_8\text{S}_2^{905}$

### Compound Data

<b>Molecular weight</b>	216.322	<b>H bond acceptors</b>	0	<b>Rule of 5 violations</b>	0
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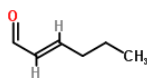


<b>Compound type</b>	non-Ugi related	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	4.57
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	0	<b>Predicted density</b>	1.31 g/cm <sup>3</sup>
<b>SMILES</b>	S1c3c(Sc2c1cccc2)cccc3				
<b>InChIKey</b>	GVIIJXMXTUZIOD-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-decanol	0.04	0.01	1.05
1,4-dioxane	0.27	0.02	6.14
acetonitrile	0.02	0.00	0.58
decane	0.03	0.01	0.89
diethyl ether	0.08	0.01	2.39
diisopropyl ether	0.05	0.01	1.44
ethylene glycol	0.02	0.00	0.40
hexadecane	0.03	0.01	0.84
nonane	0.03	0.01	0.90
undecane	0.03	0.01	0.88

### trans-2-hexen-1-al C<sub>6</sub>H<sub>10</sub>O<sup>22</sup>



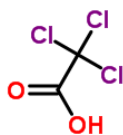
<b>Molecular weight</b>	98.143	<b>H bond acceptors</b>	1	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0	<b>ACD/ALogP</b>	1.58
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	3	<b>Predicted density</b>	0.828 g/cm <sup>3</sup>
<b>SMILES</b>	CCCC=CC=O				
<b>InChIKey</b>	MBDOYVRWFFCFHM-SNAWJCMRSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.62	□	□

□ Solute is very soluble/miscible, conversion fail.

### trichloroacetic acid C<sub>2</sub>HCl<sub>3</sub>O<sub>2</sub><sup>22</sup>



<b>Molecular weight</b>	163.387	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	1.67
<b>Phase 25°C</b>	liquid	<b>Rotatable bonds</b>	0	<b>Predicted density</b>	1.807 g/cm <sup>3</sup>
<b>SMILES</b>	C(=O)(C(Cl)(Cl)Cl)O				
<b>InChIKey</b>	YNJBWRMUSHSURL-UHFFFAOYSA-N				

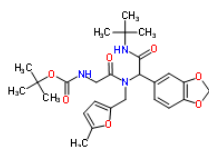
#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.91	0.80	2068.61

### UCExp216-3A C<sub>26</sub>H<sub>35</sub>N<sub>3</sub>O<sub>7</sub><sup>113</sup>

#### Compound Data

<b>Molecular weight</b>	501.572	<b>H bond acceptors</b>	10	<b>Rule of 5 violations</b>	2
<b>Compound type</b>	Ugi Product	<b>H bond donors</b>	2	<b>ACD/ALogP</b>	4.06

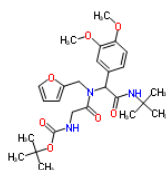


<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	10	<b>Predicted density</b>	1.209 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>CC(C)(C)NC(=O)C(c1ccc2OCOe2c1)N(Cc3ccc(C)o3)C(=O)CNC(=O)OC(C)(C)C</chem>				
<b>InChIKey</b>	MTSJLRXXXJHLDI-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
acetonitrile	0.04	0.00	2.73
DMSO	0.28	0.02	14.46
ethanol	0.03	0.00	1.95
methanol	0.06	0.00	4.10
toluene	0.01	0.00	0.58

### Ugi product 104C (UC) C<sub>26</sub>H<sub>37</sub>N<sub>3</sub>O<sub>7</sub><sup>65</sup>



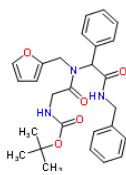
#### Compound Data

<b>Molecular weight</b>	503.588	<b>H bond acceptors</b>	10	<b>Rule of 5 violations</b>	2
<b>Compound type</b>	Ugi Product	<b>H bond donors</b>	2	<b>ACD/ALogP</b>	3.48
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	12	<b>Predicted density</b>	1.156 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>O=C(CNC(=O)OC(C)(C)C)N(Ce1ccc1)C(c2ccc(OC)c(OC)c2)C(=O)NC(C)(C)C</chem>				
<b>InChIKey</b>	RXLIYJRDQONCRV-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
methanol	0.29	0.01	22.20

### Ugi product 108C (UC) C<sub>27</sub>H<sub>31</sub>N<sub>3</sub>O<sub>5</sub><sup>65</sup>



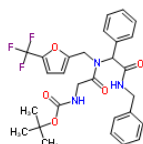
#### Compound Data

<b>Molecular weight</b>	477.552	<b>H bond acceptors</b>	8	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	Ugi Product	<b>H bond donors</b>	2	<b>ACD/ALogP</b>	4.43
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	11	<b>Predicted density</b>	1.198 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>O=C(CNC(=O)OC(C)(C)C)N(Ce1ccc1)C(c2ccc2)C(=O)NCc3ccccc3</chem>				
<b>InChIKey</b>	COBIEQVPXUIPRH-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
methanol	0.36	0.02	26.66

### Ugi product 109C(UC) C<sub>28</sub>H<sub>30</sub>F<sub>3</sub>N<sub>3</sub>O<sub>5</sub><sup>65</sup>



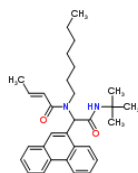
#### Compound Data

<b>Molecular weight</b>	545.55	<b>H bond acceptors</b>	8	<b>Rule of 5 violations</b>	1
<b>Compound type</b>	Ugi Product	<b>H bond donors</b>	2	<b>ACD/ALogP</b>	5
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	11	<b>Predicted density</b>	1.263 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>O=C(CNC(=O)OC(C)(C)C)N(Ce1ccc(o1)C(F)(F)F)C(c2ccccc2)C(=O)NCc3ccccc3</chem>				
<b>InChIKey</b>	XRHVZVZVUCGMHPN-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.15	0.01	11.62

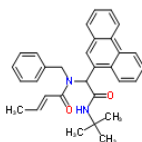
### Ugi product 148B C<sub>31</sub>H<sub>40</sub>N<sub>2</sub>O<sub>2</sub><sup>96, 145</sup>



Compound Data			
<b>Molecular weight</b>	472.661	<b>H bond acceptors</b>	4
<b>Compound type</b>	Ugi Product	<b>H bond donors</b>	1
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	11
<b>SMILES</b>	<chem>CC(C)(C)NC(=O)C(N(CCCCCC)C(=O))C=C(C)c2cc3ccccc3c1ccccc12</chem>		
<b>InChIKey</b>	HOKCUULFCASAQT-FRKPEAEDSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.02	0.00	1.28
benzene	0.05	0.00	2.77
ethanol	0.00	0.00	0.00
methanol	0.03	0.00	1.91
THF	0.4	0.04	25.03
toluene	0.14	0.02	8.10

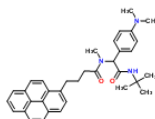
### Ugi product 150D(UC) C<sub>31</sub>H<sub>32</sub>N<sub>2</sub>O<sub>2</sub><sup>78, 65</sup>



Compound Data			
<b>Molecular weight</b>	464.598	<b>H bond acceptors</b>	4
<b>Compound type</b>	Ugi Product	<b>H bond donors</b>	1
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	7
<b>SMILES</b>	<chem>CC(C)(C)NC(=O)C(N(Cc1ccccc1)C(=O))C=C(C)c3cc4ccccc4c2ccccc23</chem>		
<b>InChIKey</b>	PBZQTKRWYXTXIS-WLRTZDKTSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.04	0.00	2.53
DMSO	0.18	0.01	8.21
ethanol	0.04	0.00	2.42
methanol	0.07	0.00	4.12
THF	0.49	0.05	31.41
toluene	0.04	0.00	2.17

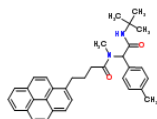
### Ugi product 171K (UC) C<sub>35</sub>H<sub>39</sub>N<sub>3</sub>O<sub>2</sub><sup>65</sup>



Compound Data			
<b>Molecular weight</b>	533.703	<b>H bond acceptors</b>	5
<b>Compound type</b>	Ugi Product	<b>H bond donors</b>	1
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	9
<b>SMILES</b>	<chem>CN(C)c1ccc(cc1)C(C(=O)NC(C)(C)N(C)C(=O))CCc5ccc4ccc3ccccc2ccc5c4c23</chem>		
<b>InChIKey</b>	XWJCEFGKUMNBLK-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.02	0.00	1.43

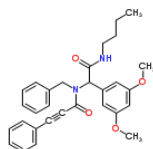
### Ugi product 173B (UC) C<sub>34</sub>H<sub>36</sub>N<sub>2</sub>O<sub>2</sub><sup>65</sup>



Compound Data			
<b>Molecular weight</b>	504.662	<b>H bond acceptors</b>	4
<b>Compound type</b>	Ugi Product	<b>H bond donors</b>	1
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	8
<b>SMILES</b>	<chem>CC(C)(C)NC(=O)C(N(C)C(=O)CCCc4ccc3ccc2cccc1ccc4c3c12)c5ccc(C)cc5</chem>		
<b>InChIKey</b>	KNHNINYGWDFMQZ-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.08	0.00	5.55

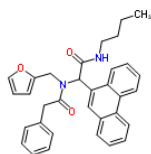
### Ugi product 173G (UC) C<sub>30</sub>H<sub>32</sub>N<sub>2</sub>O<sub>4</sub><sup>65</sup>



Compound Data			
<b>Molecular weight</b>	484.586	<b>H bond acceptors</b>	6
<b>Compound type</b>	Ugi Product	<b>H bond donors</b>	1
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	11
<b>SMILES</b>	<chem>COc1cc(cc(OC)c1)C(C(=O)NCCCC)N(Cc2ccccc2)C(=O)C#Cc3ccccc3</chem>		
<b>InChIKey</b>	VOGZWAORWZGOTE-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.18	0.01	12.50

### Ugi product 176C (UC) C<sub>33</sub>H<sub>32</sub>N<sub>2</sub>O<sub>3</sub><sup>127, 145, 65</sup>



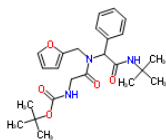
Compound Data			
<b>Molecular weight</b>	504.619	<b>H bond acceptors</b>	5
<b>Compound type</b>	Ugi Product	<b>H bond donors</b>	1
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	10
<b>SMILES</b>	<chem>O=C(Cc1ccccc1)N(Cc2ccco2)C(c4cc5ccccc5c3ccccc34)C(=O)NCCCC</chem>		
<b>InChIKey</b>	RGGYLRDGAJICY-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1,4-dioxane	0.19	0.02	10.47
acetonitrile	0.02	0.00	1.36
benzene	0.03	0.00	1.76
diethyl ether	0.02	0.00	1.39
DMF	0.27	0.02	17.67
DMSO	0.19	0.01	9.48
ethanol	0.01	0.00	0.65
methanol	0.05	0.00	3.42
THF	0.28	0.02	17.72
toluene	0.03	0.00	1.76

### Ugi product 206B(UC) C<sub>24</sub>H<sub>33</sub>N<sub>3</sub>O<sub>5</sub><sup>56</sup>

Compound Data			
<b>Molecular weight</b>	443.536	<b>H bond acceptors</b>	8
<b>Compound type</b>	Ugi Product	<b>H bond donors</b>	2
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	10
<b>SMILES</b>	<chem>CC(C)NC(=O)C(N(C)C(=O)CCCc4ccc3ccc2cccc1ccc4c3c12)c5ccc(C)cc5</chem>		
<b>InChIKey</b>	KNHNINYGWDFMQZ-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.08	0.00	5.55



**SMILES**

O=C(CNC(=O)OC(C)(C)C)N(Cc1ccco1)C(c2ccccc2)C(=O)NC(C)(C)C

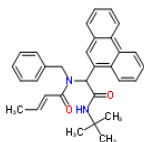
**InChIKey**

BXAOUWIVXLQYOZ-UHFFFAOYSA-N

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
2-propanol	0.00	0.00	0.00
acetonitrile	0.02	0.00	1.20
benzene	0.01	0.00	0.51
carbon tetrachloride	0.00	0.00	0.00
chloroform	0.57	0.06	21.63
cyclohexane	0.00	0.00	0.00
cyclopentane	0.00	0.00	0.00
dichloromethane	0.24	0.02	9.37
diethyl ether	0.00	0.00	0.00
DMF	0.24	0.02	13.49
DMSO	0.23	0.02	10.19
ethanol	0.02	0.00	1.15
hexane	0.00	0.00	0.00
methanol	0.05	0.00	3.00
THF	0.26	0.02	14.19
toluene	0.01	0.00	0.51

### Ugi product 214C(UC) C<sub>31</sub>H<sub>32</sub>N<sub>2</sub>O<sub>2</sub><sup>27</sup>



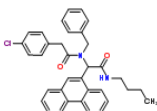
#### Compound Data

<b>Molecular weight</b>	464.598	<b>H bond acceptors</b>	4	<b>Rule of 5 violations</b>	1
<b>Compound type</b>	Ugi Product	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	6.18
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	7	<b>Predicted density</b>	1.148 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>CC(C)(C)NC(=O)C(N(Cc1ccccc1)C(=O)C=C\C)c3cc4ccccc4c2ccccc23</chem>				
<b>InChIKey</b>	PBZQTKRWYXTXIS-WLRTZDKTSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
methanol	0.01	0.00	0.62
THF	0.35	0.03	20.96

### Ugi product 215F(UC) C<sub>35</sub>H<sub>33</sub>ClN<sub>2</sub>O<sub>2</sub><sup>71</sup>



#### Compound Data

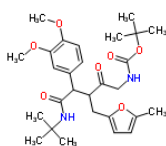
<b>Molecular weight</b>	549.102	<b>H bond acceptors</b>	4	<b>Rule of 5 violations</b>	2
<b>Compound type</b>	Ugi Product	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	8.33
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	10	<b>Predicted density</b>	1.219 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>Clc5ccc(CC(=O)N(Cc1ccccc1)C(c3cc4ccccc4c2ccccc23)C(=O)NCCCC)cc5</chem>				
<b>InChIKey</b>	NCOSMKWGNCPJCR-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	p <sub>ph</sub> (g/100g)
acetonitrile	0.04	0.00	2.99
DMSO	0.38	0.03	22.91
ethanol	0.06	0.00	4.34
methanol	0.12	0.01	9.25

THF	0.61	0.06	51.09
toluene	0.07	0.01	4.56

## Ugi Product 216-4A C<sub>28</sub>H<sub>40</sub>N<sub>2</sub>O<sub>7</sub><sup>93, 97</sup>



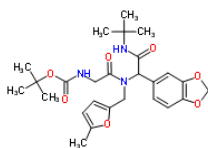
<b>Molecular weight</b>	516.626	<b>H bond acceptors</b>	9	<b>Rule of 5 violations</b>	1
<b>Compound type</b>	Ugi Product	<b>H bond donors</b>	2	<b>ACD/ALogP</b>	4.08
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	13	<b>Predicted density</b>	1.12 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>Cc1ccc(o1)CC(C(c2ccc(c(c2)OC)OC)C(=O)NC(C)(C)C)C(=O)CNC(=O)OC(C)(C)C</chem>				
<b>InChIKey</b>					

### Compound Data

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.13	0.01	9.17
DMSO	0.06	0.00	2.90
ethanol	0.07	0.00	4.79
methanol	0.18	0.01	13.47
toluene	0.2	0.02	13.07

## Ugi product 62E (UC) C<sub>26</sub>H<sub>35</sub>N<sub>3</sub>O<sub>7</sub><sup>65</sup>



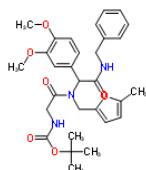
<b>Molecular weight</b>	501.572	<b>H bond acceptors</b>	10	<b>Rule of 5 violations</b>	2
<b>Compound type</b>	Ugi Product	<b>H bond donors</b>	2	<b>ACD/ALogP</b>	4.06
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	10	<b>Predicted density</b>	1.209 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>CC(C)(C)NC(=O)c(c1ccc2OCOc2e1)N(Cc3ccc(C)o3)C(=O)CNC(=O)OC(C)(C)C</chem>				
<b>InChIKey</b>	MTSJLRXXXJHLDI-UHFFFAOYSA-N				

### Compound Data

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.13	0.01	9.15

## Ugi product 64C (UC) C<sub>30</sub>H<sub>37</sub>N<sub>3</sub>O<sub>7</sub><sup>65</sup>



<b>Molecular weight</b>	551.631	<b>H bond acceptors</b>	10	<b>Rule of 5 violations</b>	2
<b>Compound type</b>	Ugi Product	<b>H bond donors</b>	2	<b>ACD/ALogP</b>	4.63
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	13	<b>Predicted density</b>	1.192 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>CC(C)(C)OC(=O)NCC(=O)N(Cc1ccc(C)o1)C(C(=O)NCc2ccccc2)c3ccc(OC)c(OC)c3</chem>				
<b>InChIKey</b>	VMMFSZQZVZNXS-K-UHFFFAOYSA-N				

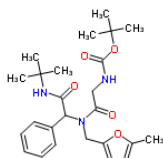
### Compound Data

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.03	0.00	2.23

## Ugi product 86B (UC) C<sub>25</sub>H<sub>35</sub>N<sub>3</sub>O<sub>5</sub><sup>65</sup>

### Compound Data

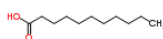


<b>Molecular weight</b>	457.562	<b>H bond acceptors</b>	8	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	Ugi Product	<b>H bond donors</b>	2	<b>ACD/ALogP</b>	4.2
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	10	<b>Predicted density</b>	1.133 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>O=C(CNC(=O)OC(C)(C)C)N(Cc1ccc(C)cc1)C(c2ccccc2)C(=O)NC(C)(C)C</chem>				
<b>InChIKey</b>	WDAGUORBKBNETC-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.17	0.01	11.09

### undecanoic acid C<sub>11</sub>H<sub>22</sub>O<sub>2</sub><sup>58</sup>



<b>Molecular weight</b>	186.291	<b>H bond acceptors</b>	2	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	carboxylic acid	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	4.5
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	9	<b>Predicted density</b>	0.909 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>O=C(O)CCCCCCCCCC</chem>				
<b>InChIKey</b>	ZDPHROEEEOARMN-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	3.94	0.55	488.75
methanol	4	0.49	549.05

### urea CH<sub>4</sub>N<sub>2</sub>O<sup>53</sup>

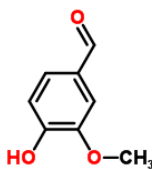


<b>Molecular weight</b>	60.0553	<b>H bond acceptors</b>	3	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	amide	<b>H bond donors</b>	4	<b>ACD/ALogP</b>	-2.11
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	0	<b>Predicted density</b>	1.212 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>NC(=O)N</chem>				
<b>InChIKey</b>	XSQUKJJFZCRTK-UHFFFAOYSA-N				

#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	2.66	0.12	24.44

### vanillin C<sub>8</sub>H<sub>8</sub>O<sub>3</sub><sup>906, 4, 10, 11, 55, 207, 19</sup>



<b>Molecular weight</b>	152.147	<b>H bond acceptors</b>	3	<b>Rule of 5 violations</b>	0
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	1	<b>ACD/ALogP</b>	1.19
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	3	<b>Predicted density</b>	1.231 g/cm <sup>3</sup>
<b>SMILES</b>	<chem>Oc1ccc(cc1OC)C=O</chem>				
<b>InChIKey</b>	MWOOGOJBHIARFG-UHFFFAOYSA-N				

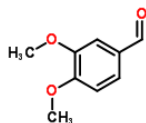
#### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-propanol	1.82	0.15	44.94
1,2-dichloroethane	1.17	0.10	17.74
acetonitrile	2.36	0.15	67.86
butanone	2.14	0.21	56.32



ethanol	2.47	0.17	69.35
methanol	4.16	0.27	173.01
THF	3.6	0.34	108.89
toluene	0.3	0.03	5.44

## veratraldehyde C<sub>9</sub>H<sub>10</sub>O<sub>3</sub><sup>41, 71, 208</sup>

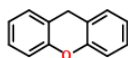


Compound Data			
<b>Molecular weight</b>	166.174	<b>H bond acceptors</b>	3
<b>Compound type</b>	aldehyde	<b>H bond donors</b>	0
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	3
<b>SMILES</b>	COc1cc(ccc1OC)C=O		
<b>InChIKey</b>	WJUFSDZVCOTFON-UHFFFAOYSA-N		
<b>Rule of 5 violations</b>	0	<b>ACD/ALogP</b>	1.61
<b>Predicted density</b>	1.114 g/cm <sup>3</sup>		

### Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetone	3.03	0.29	119.01
acetonitrile	5.76	0.69	904.54
chloroform	5.7	0.75	421.71
dichloromethane	6.06	0.81	837.51
diethyl ether	3.55	0.43	170.84
DMSO	5.31	0.64	386.17
ethanol	5.49	0.64	645.97
hexane	0.07	0.01	1.74
methanol	5.87	0.67	1041.50
THF	5.34	0.68	480.29
toluene	4.54	0.60	267.44

## xanthene C<sub>13</sub>H<sub>10</sub>O<sup>905</sup>



Compound Data			
<b>Molecular weight</b>	182.218	<b>H bond acceptors</b>	1
<b>Compound type</b>	non-Ugi related	<b>H bond donors</b>	0
<b>Phase 25°C</b>	solid	<b>Rotatable bonds</b>	0
<b>SMILES</b>	O2c1ccccc1Cc3c2cccc3		
<b>InChIKey</b>	GJCOSYZMQJWQCA-UHFFFAOYSA-N		
<b>Rule of 5 violations</b>	0	<b>ACD/ALogP</b>	3.93
<b>Predicted density</b>	1.159 g/cm <sup>3</sup>		

### Solubility Data

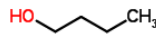
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.19	0.02	4.43
1-decanol	0.24	0.05	5.49
1-heptanol	0.23	0.03	5.30
1-hexanol	0.22	0.03	5.09
1-octanol	0.24	0.04	5.52
1-pentanol	0.2	0.02	4.64
1-propanol	0.15	0.01	3.52
1,2-dichloroethane	1.62	0.15	33.77
2-butanol	0.13	0.01	3.02
2-methyl-1-pentanol	0.16	0.02	3.67
2-methyl-1-propanol	0.12	0.01	2.78
2-methyl-2-butanol	0.18	0.02	4.16
2-methyl-2-propanol	0.12	0.01	2.77
2-pentanol	0.16	0.02	3.70
2-propanol	0.11	0.01	2.58
2,2,4-trimethylpentane	0.15	0.02	3.95
3-methyl-1-butanol	0.15	0.02	3.46
4-methyl-2-pentanol	0.14	0.02	3.22

acetonitrile	0.35	0.02	9.03
carbon tetrachloride	1.25	0.12	16.71
cyclohexane	0.39	0.04	9.58
cyclooctane	0.38	0.05	9.32
cyclopentanol	0.33	0.03	6.32
decane	0.24	0.05	6.19
dibutyl ether	0.5	0.08	12.68
diethyl ether	0.79	0.08	22.39
diisopropyl ether	0.41	0.06	10.54
ethanol	0.1	0.01	2.37
heptane	0.24	0.03	6.54
hexadecane	0.24	0.07	5.88
hexane	0.23	0.03	6.44
methanol	0.1	0.00	2.46
methyl tert-butyl ether	0.65	0.08	17.59
methylcyclohexane	0.33	0.04	8.17
nonane	0.24	0.04	6.28
octane	0.25	0.04	6.67
undecane	0.23	0.05	5.85

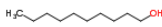
## Solvents

Below we present data for the solvents used in the Open Notebook Science Challenge. We present various properties such as density and boiling point together with important solvation related parameters such as dielectric constants and dipole moments [1000-1100].

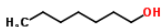
### 1-butanol

Compound Data	
	<b>Molecular weight</b> 74.1216
	<b>Predicted density</b> 0.805 g/cm <sup>3</sup>
	<b>Boiling point</b> 117.7 °C
	<b>Dipole moment</b> 1.66
	<b>Dielectric constant</b> 17.8
	<b>SMILES</b> CCCC
	<b>InChIKey</b> LRHPLDGYMQRHN-UHFFFAOYSA-N

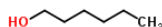
### 1-decanol

Compound Data	
	<b>Molecular weight</b> 158.2811
	<b>Predicted density</b> 0.828 g/cm <sup>3</sup>
	<b>Boiling point</b> 227.8 °C
	<b>SMILES</b> OCCCCCCCCC
	<b>InChIKey</b> MWKFXSUHHTGQN-UHFFFAOYSA-N

### 1-heptanol

Compound Data	
	<b>Molecular weight</b> 116.2013
	<b>Predicted density</b> 0.82 g/cm <sup>3</sup>
	<b>Boiling point</b> 176.9 °C
	<b>SMILES</b> OCCCCCC
	<b>InChIKey</b> BBMCTIGTCKYKF-UHFFFAOYSA-N

## 1-hexanol



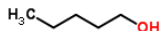
Compound Data	
Molecular weight	102.1748
Predicted density	0.816 g/cm <sup>3</sup>
Boiling point	158.2 °C
Dipole moment	1.55
Dielectric constant	13.3
SMILES	OCCCCC
InChIKey	ZSIAUFGUXNUGDI-UHFFFAOYSA-N

## 1-octanol



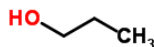
Compound Data	
Molecular weight	130.2279
Predicted density	0.823 g/cm <sup>3</sup>
Boiling point	194.7 °C
SMILES	OCCCCCCC
InChIKey	KBPLFHHGFOOTCA-UHFFFAOYSA-N

## 1-pentanol



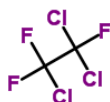
Compound Data	
Molecular weight	88.1482
Predicted density	0.811 g/cm <sup>3</sup>
Boiling point	138.5 °C
SMILES	OCCCC
InChIKey	AMQJEAYHLZJPGS-UHFFFAOYSA-N

## 1-propanol



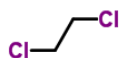
Compound Data	
Molecular weight	60.095
Predicted density	0.795 g/cm <sup>3</sup>
Boiling point	95.8 °C
Dipole moment	1.68
Dielectric constant	20.1
SMILES	CCCO
InChIKey	BDERNNFJNOPAEC-UHFFFAOYSA-N

## 1,1,2-trichlorotrifluoroethane



Compound Data	
Molecular weight	187.3756
Predicted density	1.67 g/cm <sup>3</sup>
Boiling point	50.9 °C
SMILES	ClC(F)(F)C(Cl)(Cl)F
InChIKey	AJDIZQLSFPQPEY-UHFFFAOYSA-N

## 1,2-dichloroethane



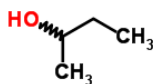
Compound Data	
Molecular weight	98.9592
Predicted density	1.173 g/cm <sup>3</sup>
Boiling point	83.5 °C
SMILES	ClCCCl
InChIKey	WSLDOOZREJYCGB-UHFFFAOYSA-N

## 1,4-dioxane



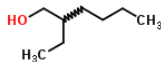
Compound Data	
Molecular weight	88.1051
Predicted density	0.995 g/cm <sup>3</sup>
Boiling point	102.9 °C
SMILES	O1CCOCC1
InChIKey	RYHBNJHYFVUHQT-UHFFFAOYSA-N

## 2-butanol



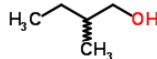
Compound Data	
Molecular weight	74.1216
Predicted density	0.801 g/cm <sup>3</sup>
Boiling point	96.6 °C
SMILES	OC(C)CC
InChIKey	BTANRVKQNVYAZ-UHFFFAOYSA-N

## 2-ethyl-1-hexanol



Compound Data	
Molecular weight	130.2279
Predicted density	0.821 g/cm <sup>3</sup>
Boiling point	184.6 °C
SMILES	OCC(CC)CCCC
InChIKey	YIWUKEYIRIRTPP-UHFFFAOYSA-N

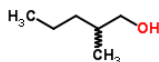
## 2-methyl-1-butanol



Compound Data	
Molecular weight	88.1482
Predicted density	0.809 g/cm <sup>3</sup>
Boiling point	128.7 °C
SMILES	OCC(C)CC
InChIKey	QPRQEDXDYOZYLA-UHFFFAOYSA-N

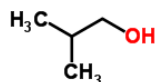
## 2-methyl-1-pentanol

Compound Data	
Molecular weight	102.1748
Predicted density	0.814 g/cm <sup>3</sup>



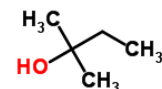
<b>Boiling point</b>	148 °C
<b>SMILES</b>	OCC(C)CC
<b>InChIKey</b>	PFNHSEQQEPMLNI-UHFFFAOYSA-N

## 2-methyl-1-propanol



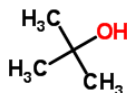
Compound Data	
<b>Molecular weight</b>	74.1216
<b>Predicted density</b>	0.801 g/cm <sup>3</sup>
<b>Boiling point</b>	105 °C
<b>SMILES</b>	OCC(C)C
<b>InChIKey</b>	ZXEKIIIBDNHEJQC-UHFFFAOYSA-N

## 2-methyl-2-butanol



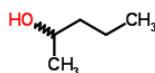
Compound Data	
<b>Molecular weight</b>	88.1482
<b>Predicted density</b>	0.811 g/cm <sup>3</sup>
<b>Boiling point</b>	102 °C
<b>SMILES</b>	OC(C)(C)CC
<b>InChIKey</b>	MSXVEPNJUHWQHW-UHFFFAOYSA-N

## 2-methyl-2-propanol



Compound Data	
<b>Molecular weight</b>	74.1216
<b>Predicted density</b>	0.804 g/cm <sup>3</sup>
<b>Boiling point</b>	84.6 °C
<b>SMILES</b>	OC(C)(C)C
<b>InChIKey</b>	DKGAVHZHDRPRBM-UHFFFAOYSA-N

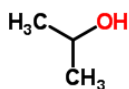
## 2-pentanol



Compound Data	
<b>Molecular weight</b>	88.1482
<b>Predicted density</b>	0.809 g/cm <sup>3</sup>
<b>Boiling point</b>	118.8 °C
<b>SMILES</b>	OC(C)CCC
<b>InChIKey</b>	JYVLIDXNZAXMDK-UHFFFAOYSA-N

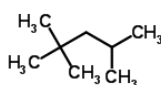
## 2-propanol

Compound Data	
<b>Molecular weight</b>	60.095
<b>Predicted density</b>	0.791 g/cm <sup>3</sup>
<b>Boiling point</b>	73 °C



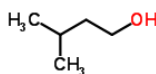
<b>Dipole moment</b>	1.66
<b>Dielectric constant</b>	1.89
<b>SMILES</b>	CC(O)C
<b>InChIKey</b>	KFZMGEQAYNKOFK-UHFFFAOYSA-N

## 2,2,4-trimethylpentane



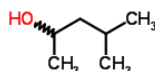
Compound Data	
<b>Molecular weight</b>	114.2285
<b>Predicted density</b>	0.709 g/cm <sup>3</sup>
<b>Boiling point</b>	98.8 °C
<b>SMILES</b>	CC(C)CC(C)(C)C
<b>InChIKey</b>	NHTMVDHEPJAVLT-UHFFFAOYSA-N

## 3-methyl-1-butanol



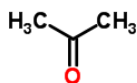
Compound Data	
<b>Molecular weight</b>	88.1482
<b>Predicted density</b>	0.809 g/cm <sup>3</sup>
<b>Boiling point</b>	131.2 °C
<b>SMILES</b>	OCCC(C)C
<b>InChIKey</b>	PHTQWCKDNZKARW-UHFFFAOYSA-N

## 4-methyl-2-pentanol



Compound Data	
<b>Molecular weight</b>	102.1748
<b>Predicted density</b>	0.811 g/cm <sup>3</sup>
<b>Boiling point</b>	133.5 °C
<b>SMILES</b>	OC(C)CC(C)C
<b>InChIKey</b>	WVYWICLMDOOCFB-UHFFFAOYSA-N

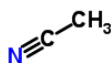
## acetone



Compound Data	
<b>Molecular weight</b>	58.0791
<b>Predicted density</b>	0.772 g/cm <sup>3</sup>
<b>Boiling point</b>	46.5 °C
<b>Dipole moment</b>	2.88
<b>Dielectric constant</b>	20.7
<b>SMILES</b>	CC(=O)C
<b>InChIKey</b>	CSCPPACGZOOXG-UHFFFAOYSA-N

## acetonitrile

### Compound Data



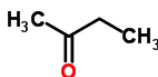
<b>Molecular weight</b>	41.0519
<b>Predicted density</b>	0.747 g/cm <sup>3</sup>
<b>Boiling point</b>	63.5 °C
<b>Dipole moment</b>	3.92
<b>Dielectric constant</b>	36.6
<b>SMILES</b>	CCN
<b>InChIKey</b>	QUSNBJAOOMFDIB-UHFFFAOYSA-N

## benzene



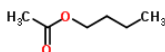
Compound Data	
<b>Molecular weight</b>	78.1118
<b>Predicted density</b>	0.873 g/cm <sup>3</sup>
<b>Boiling point</b>	78.8 °C
<b>Dipole moment</b>	0
<b>Dielectric constant</b>	2.28
<b>SMILES</b>	c1ccccc1
<b>InChIKey</b>	UHOVQNZJYSORNB-UHFFFAOYSA-N

## butanone



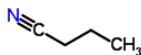
Compound Data	
<b>Molecular weight</b>	72.1057
<b>Predicted density</b>	0.786 g/cm <sup>3</sup>
<b>Boiling point</b>	75.6 °C
<b>SMILES</b>	O=C(C)CC
<b>InChIKey</b>	ZWEHNKRNPVVGH-UHFFFAOYSA-N

## butyl acetate



Compound Data	
<b>Molecular weight</b>	116.1583
<b>Predicted density</b>	0.886 g/cm <sup>3</sup>
<b>Boiling point</b>	126.6 °C
<b>SMILES</b>	O=C(OCCCC)C
<b>InChIKey</b>	DKPFZGUDAPQIHT-UHFFFAOYSA-N

## butyronitrile



Compound Data	
<b>Molecular weight</b>	69.1051
<b>Predicted density</b>	0.785 g/cm <sup>3</sup>
<b>Boiling point</b>	117.3 °C
<b>SMILES</b>	N#CCCC
<b>InChIKey</b>	KVNRLNFWIYMESJ-UHFFFAOYSA-N

## carbon disulfide

### Compound Data



<b>Molecular weight</b>	76.1407
<b>Predicted density</b>	1.259 g/cm <sup>3</sup>
<b>Boiling point</b>	46.2 °C
<b>SMILES</b>	S=C=S
<b>InChIKey</b>	QGJOPFRUJISHPQ-UHFFFAOYSA-N

## carbon tetrachloride



Compound Data	
<b>Molecular weight</b>	153.8227
<b>Predicted density</b>	1.697 g/cm <sup>3</sup>
<b>Boiling point</b>	76 °C
<b>Dipole moment</b>	0
<b>Dielectric constant</b>	2.24
<b>SMILES</b>	[C](Cl)(Cl)(Cl)Cl
<b>InChIKey</b>	VZGDMQKNWNREIO-UHFFFAOYSA-N

## chloroform



Compound Data	
<b>Molecular weight</b>	119.3776
<b>Predicted density</b>	1.5 g/cm <sup>3</sup>
<b>Boiling point</b>	61.2 °C
<b>Dipole moment</b>	1.15
<b>Dielectric constant</b>	5.5
<b>SMILES</b>	C(Cl)(Cl)Cl
<b>InChIKey</b>	HEDRZPFGACZZDS-UHFFFAOYSA-N

## cyclohexane



Compound Data	
<b>Molecular weight</b>	84.1595
<b>Predicted density</b>	0.79 g/cm <sup>3</sup>
<b>Boiling point</b>	80.7 °C
<b>Dipole moment</b>	0
<b>Dielectric constant</b>	18.5
<b>SMILES</b>	C1CCCCC1
<b>InChIKey</b>	XDTMQSROBMDMFD-UHFFFAOYSA-N

## cyclooctane



Compound Data	
<b>Molecular weight</b>	112.2126
<b>Predicted density</b>	0.79 g/cm <sup>3</sup>
<b>Boiling point</b>	152 °C
<b>SMILES</b>	C1CCCCCCC1
<b>InChIKey</b>	WJTCGQSWYFHTAC-UHFFFAOYSA-N



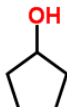
## cyclopentane



### Compound Data

<b>Molecular weight</b>	70.1329
<b>Predicted density</b>	0.79 g/cm <sup>3</sup>
<b>Boiling point</b>	49.2 °C
<b>SMILES</b>	C1CCCC1
<b>InChIKey</b>	RGSFGYAAUTVSQA-UHFFFAOYSA-N

## cyclopentanol



### Compound Data

<b>Molecular weight</b>	86.1323
<b>Predicted density</b>	1.004 g/cm <sup>3</sup>
<b>Boiling point</b>	140.8 °C
<b>SMILES</b>	OC1CCCC1
<b>InChIKey</b>	XCIXKGXIYUWCLL-UHFFFAOYSA-N

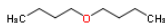
## decane



### Compound Data

<b>Molecular weight</b>	142.2817
<b>Predicted density</b>	0.734 g/cm <sup>3</sup>
<b>Boiling point</b>	174.9 °C
<b>SMILES</b>	C(CCCCCCCC)C
<b>InChIKey</b>	DIOQZVSGTUSAI-UHFFFAOYSA-N

## dibutyl ether



### Compound Data

<b>Molecular weight</b>	130.2279
<b>Predicted density</b>	0.78 g/cm <sup>3</sup>
<b>Boiling point</b>	142.1 °C
<b>SMILES</b>	O(CCCC)CCCC
<b>InChIKey</b>	DURPTKYDGMDSBL-UHFFFAOYSA-N

## dichloromethane

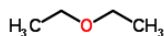


### Compound Data

<b>Molecular weight</b>	84.9326
<b>Predicted density</b>	1.252 g/cm <sup>3</sup>
<b>Boiling point</b>	39.6 °C
<b>Dipole moment</b>	1.6
<b>Dielectric constant</b>	9.08
<b>SMILES</b>	C(Cl)Cl
<b>InChIKey</b>	YMWUJEATGCHHMB-UHFFFAOYSA-N

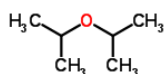
## diethyl ether

### Compound Data



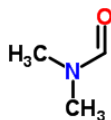
<b>Molecular weight</b>	74.1216
<b>Predicted density</b>	0.734 g/cm <sup>3</sup>
<b>Boiling point</b>	33.2 °C
<b>Dipole moment</b>	1.15
<b>Dielectric constant</b>	4.34
<b>SMILES</b>	CCOCC
<b>InChIKey</b>	RTZKZFJDLAIYFH-UHFFFAOYSA-N

## diisopropyl ether



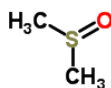
Compound Data	
<b>Molecular weight</b>	102.1748
<b>Predicted density</b>	0.758 g/cm <sup>3</sup>
<b>Boiling point</b>	68.3 °C
<b>SMILES</b>	O(C(C)C)C(C)C
<b>InChIKey</b>	ZAFNMIOTHYJRJ-UHFFFAOYSA-N

## DMF



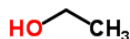
Compound Data	
<b>Molecular weight</b>	73.0938
<b>Predicted density</b>	0.87 g/cm <sup>3</sup>
<b>Boiling point</b>	153 °C
<b>Dipole moment</b>	3.82
<b>Dielectric constant</b>	38.3
<b>SMILES</b>	O=C(NC)C
<b>InChIKey</b>	OHLUHNLEMFGTQ-UHFFFAOYSA-N

## DMSO



Compound Data	
<b>Molecular weight</b>	78.1334
<b>Predicted density</b>	1.099 g/cm <sup>3</sup>
<b>Boiling point</b>	189 °C
<b>Dipole moment</b>	3.96
<b>Dielectric constant</b>	47.2
<b>SMILES</b>	CS(=O)C
<b>InChIKey</b>	IAZDPXIOMUYVGZ-UHFFFAOYSA-N

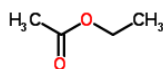
## ethanol



Compound Data	
<b>Molecular weight</b>	46.0684
<b>Predicted density</b>	0.78 g/cm <sup>3</sup>
<b>Boiling point</b>	72.6 °C
<b>Dipole moment</b>	1.69
<b>Dielectric constant</b>	24.3
<b>SMILES</b>	CCO

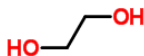
InChIKey LFQSCWFLJHTTHZ-UHFFFAOYSA-N

## ethyl acetate



Compound Data	
<b>Molecular weight</b>	88.1051
<b>Predicted density</b>	0.898 g/cm <sup>3</sup>
<b>Boiling point</b>	73.9 °C
<b>Dipole moment</b>	1.78
<b>Dielectric constant</b>	6.02
<b>SMILES</b>	CCOC(=O)C1=NN(C(=N1)C(C1)(C1)C2=C(C=C(C=C2)C1)C1
<b>InChIKey</b>	GMBRUAIJEFRHFQ-UHFFFAOYSA-N

## ethylene glycol



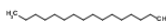
Compound Data	
<b>Molecular weight</b>	62.0678
<b>Predicted density</b>	1.097 g/cm <sup>3</sup>
<b>Boiling point</b>	197.5 °C
<b>SMILES</b>	OCCO
<b>InChIKey</b>	LYCAIKOWRPUZTN-UHFFFAOYSA-N

## heptane



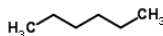
Compound Data	
<b>Molecular weight</b>	100.2019
<b>Predicted density</b>	0.695 g/cm <sup>3</sup>
<b>Boiling point</b>	98.8 °C
<b>SMILES</b>	CCCCCCC
<b>InChIKey</b>	IMNFDUFMRHMDMM-UHFFFAOYSA-N

## hexadecane



Compound Data	
<b>Molecular weight</b>	226.4412
<b>Predicted density</b>	0.773 g/cm <sup>3</sup>
<b>Boiling point</b>	286.6 °C
<b>SMILES</b>	CCCCCCCCCCCCCCCC
<b>InChIKey</b>	DCAYPVUWAIABOU-UHFFFAOYSA-N

## hexane



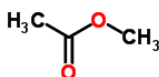
Compound Data	
<b>Molecular weight</b>	86.1754
<b>Predicted density</b>	0.675 g/cm <sup>3</sup>
<b>Boiling point</b>	68.5 °C
<b>Dipole moment</b>	0.08
<b>Dielectric constant</b>	2.02
<b>SMILES</b>	CCCCCC
<b>InChIKey</b>	VLKZOEYAKHREP-UHFFFAOYSA-N

## methanol



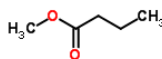
Compound Data	
Molecular weight	32.0419
Predicted density	0.753 g/cm <sup>3</sup>
Boiling point	48.1 °C
Dipole moment	1.7
Dielectric constant	33
SMILES	CO
InChIKey	OKKJLVBELUTLKV-UHFFFAOYSA-N

## methyl acetate



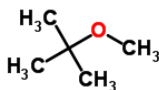
Compound Data	
Molecular weight	74.0785
Predicted density	0.908 g/cm <sup>3</sup>
Boiling point	44 °C
SMILES	CC(=O)OC
InChIKey	KKKVLQRXCPHEJC-UHFFFAOYSA-N

## methyl butyrate



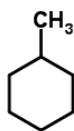
Compound Data	
Molecular weight	102.1317
Predicted density	0.891 g/cm <sup>3</sup>
Boiling point	104.2 °C
SMILES	CCCC(=O)OC
InChIKey	UUIQMZJEGPQKFD-UHFFFAOYSA-N

## methyl tert-butyl ether



Compound Data	
Molecular weight	88.1482
Predicted density	0.75 g/cm <sup>3</sup>
Boiling point	55.2 °C
SMILES	CC(C)(C)OC
InChIKey	BZLVMXJERCGZMT-UHFFFAOYSA-N


## methylcyclohexane



Compound Data	
Molecular weight	98.1861
Predicted density	0.776 g/cm <sup>3</sup>
Boiling point	101.1 °C
SMILES	CC1CCCCC1
InChIKey	UAEPNZWRGJTJPN-UHFFFAOYSA-N


## nonane

### Compound Data

	<b>Molecular weight</b>	128.2551
	<b>Predicted density</b>	0.724 g/cm <sup>3</sup>
	<b>Boiling point</b>	151.7 °C
	<b>SMILES</b>	CCCCCCCC
	<b>InChIKey</b>	BKIMMITUMNQMOS-UHFFFAOYSA-N

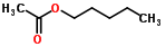
## octane

### Compound Data

	<b>Molecular weight</b>	114.2285
	<b>Predicted density</b>	0.711 g/cm <sup>3</sup>
	<b>Boiling point</b>	126.4 °C
	<b>SMILES</b>	CCCCCCCC
	<b>InChIKey</b>	

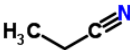
## pentyl acetate

### Compound Data

	<b>Molecular weight</b>	130.1849
	<b>Predicted density</b>	0.882 g/cm <sup>3</sup>
	<b>Boiling point</b>	149.9 °C
	<b>SMILES</b>	O=C(OCCCC)C
	<b>InChIKey</b>	PGMYKACGEOXYJE-UHFFFAOYSA-N

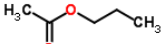
## propionitrile

### Compound Data

	<b>Molecular weight</b>	55.0785
	<b>Predicted density</b>	0.771 g/cm <sup>3</sup>
	<b>Boiling point</b>	91.3 °C
	<b>SMILES</b>	N#CCC
	<b>InChIKey</b>	FVSKHRXBFJPNKK-UHFFFAOYSA-N

## propyl acetate

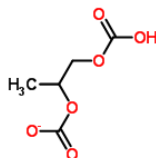
### Compound Data

	<b>Molecular weight</b>	102.1317
	<b>Predicted density</b>	0.891 g/cm <sup>3</sup>
	<b>Boiling point</b>	101.4 °C
	<b>SMILES</b>	O=C(OCCC)C
	<b>InChIKey</b>	YKYONYBAUNKHLG-UHFFFAOYSA-N

## propylene carbonate

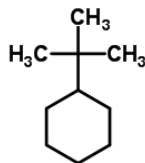
### Compound Data

<b>Molecular weight</b>	163.106
<b>Predicted density</b>	1.205 g/cm <sup>3</sup>
<b>Boiling point</b>	332.3 °C



**SMILES** OC(=O)OCC(C)OC(=O)[O-]  
**InChIKey** ZEBXBLIKXVICMJ-UHFFFAOYSA-M

### tert-butylcyclohexane



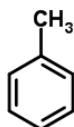
**Compound Data**  
**Molecular weight** 140.2658  
**Predicted density** 0.812 g/cm<sup>3</sup>  
**Boiling point** 168.3 °C  
**SMILES** CC(C)(C)C1CCCCC1  
**InChIKey** XTVMZZBLCLWBPM-UHFFFAOYSA-N

### THF



**Compound Data**  
**Molecular weight** 72.1057  
**Predicted density** 0.904 g/cm<sup>3</sup>  
**Boiling point** 68.3 °C  
**Dipole moment** 1.63  
**Dielectric constant** 7.52  
**SMILES** C1CCOC1  
**InChIKey** WYURNTSHIVDZCO-UHFFFAOYSA-N

### toluene



**Compound Data**  
**Molecular weight** 92.1384  
**Predicted density** 0.871 g/cm<sup>3</sup>  
**Boiling point** 110.6 °C  
**Dipole moment** 0.36  
**Dielectric constant** 2.38  
**SMILES** c1ccccc1C  
**InChIKey** YXFVVABEGXRONW-UHFFFAOYSA-N

### undecane



**Compound Data**  
**Molecular weight** 156.3083  
**Predicted density** 0.743 g/cm<sup>3</sup>  
**Boiling point** 196.3 °C  
**SMILES** C(CCCCCCCC)CC  
**InChIKey** RSJKGSCJYJTIGS-UHFFFAOYSA-N

### water

**Compound Data**



<b>Molecular weight</b>	18.0153
<b>Predicted density</b>	0.998 g/cm <sup>3</sup>
<b>Boiling point</b>	100 °C
<b>SMILES</b>	O
<b>InChIKey</b>	XLYOFNOQVPJJNP-UHFFFAOYSA-N

## References

- [1] ONS Challenge Lab Notebook Page, <http://onschallenge.wikispaces.com/JennyHale-1>
- [2] ONS Challenge Lab Notebook Page, <http://onschallenge.wikispaces.com/JennyHale-2>
- [3] ONS Challenge Lab Notebook Page, <http://onschallenge.wikispaces.com/JennyHale+3>
- [4] ONS Challenge Lab Notebook Page, <http://onschallenge.wikispaces.com/Exp004>
- [5] ONS Challenge Lab Notebook Page, <http://onschallenge.wikispaces.com/Exp005>
- [7] ONS Challenge Lab Notebook Page, <http://onschallenge.wikispaces.com/Exp007>
- [9] ONS Challenge Lab Notebook Page, <http://onschallenge.wikispaces.com/EXP009>
- [10] ONS Challenge Lab Notebook Page, <http://onschallenge.wikispaces.com/JennyHale-5>
- [11] ONS Challenge Lab Notebook Page, <http://onschallenge.wikispaces.com/JennyHale-6>
- [14] ONS Challenge Lab Notebook Page, <http://onschallenge.wikispaces.com/JennyHale-8>
- [15] ONS Challenge Lab Notebook Page, <http://onschallenge.wikispaces.com/JennyHale-9>
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- [27] ONS Challenge Lab Notebook Page, <http://onschallenge.wikispaces.com/Exp027>
- [29] ONS Challenge Lab Notebook Page, <http://onschallenge.wikispaces.com/Exp029>
- [30] ONS Challenge Lab Notebook Page, <http://onschallenge.wikispaces.com/EXP030>
- [32] ONS Challenge Lab Notebook Page, <http://onschallenge.wikispaces.com/JennyHale-11>
- [33] ONS Challenge Lab Notebook Page, <http://onschallenge.wikispaces.com/Exp033>
- [34] ONS Challenge Lab Notebook Page, <http://onschallenge.wikispaces.com/EXP034>
- [35] ONS Challenge Lab Notebook Page, <http://onschallenge.wikispaces.com/Exp035>
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