The Library

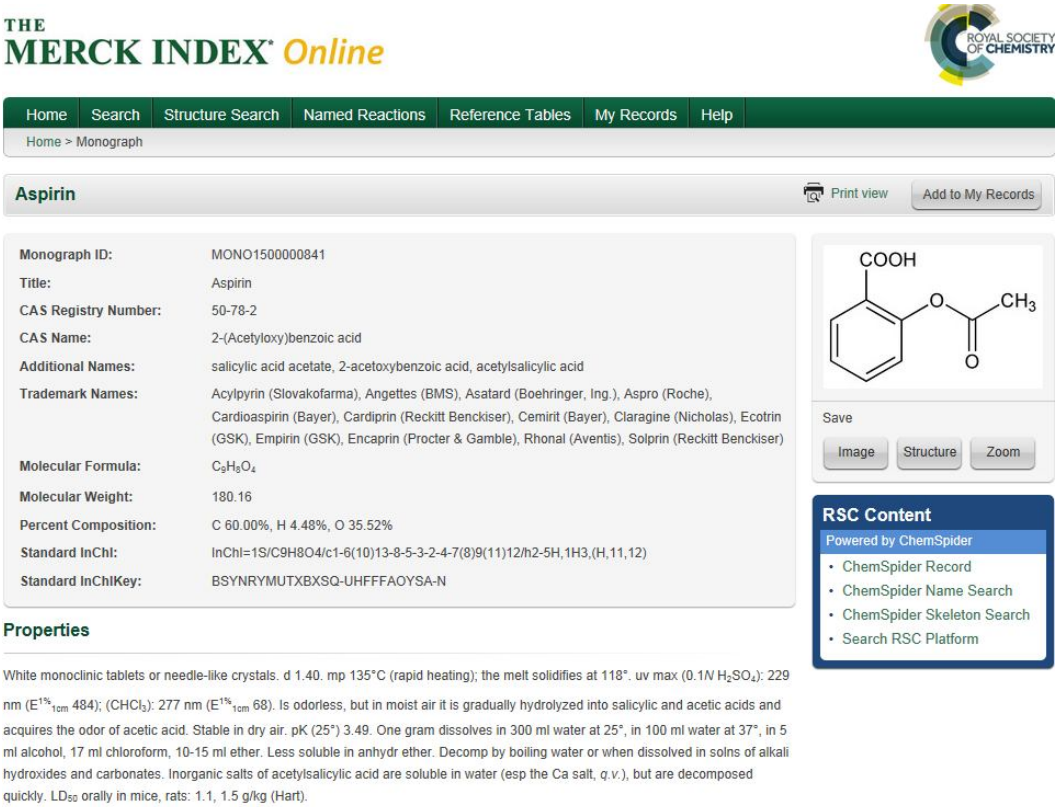
Finding chemical and physical property data

There are so many sources of chemical and physical property data that it's difficult to know where to start. This guide highlights a few of the resources that we have available through the University of Bath Library plus a few key open access resources. The resources are all listed on the library webpage for chemistry: http://www.bath.ac.uk/library/subjects/chem/index.html

Measurements of physical and chemical properties are often done by researchers in academic institutions and published in the journal literature. Governments and chemical companies also produce property data. Individual measurements may vary due to factors such as temperature, pressure and purity of the substance. For common substances, properties will have been measured many times and an 'accepted value' will be entered into a data compendium. These are the best places to start your search.

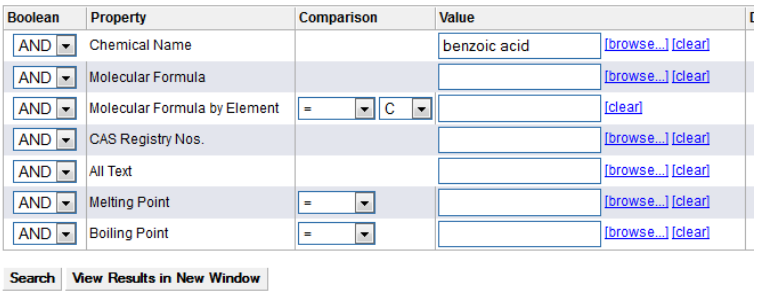
Merck Index

Hosted by the RSC, it contains information on over 11,500 substances. Includes melting point, boiling point, density and solubility. Also gives the chemical structure and literature references to synthesis and bioactivity. Search by name, formula, CAS registry number or structure.



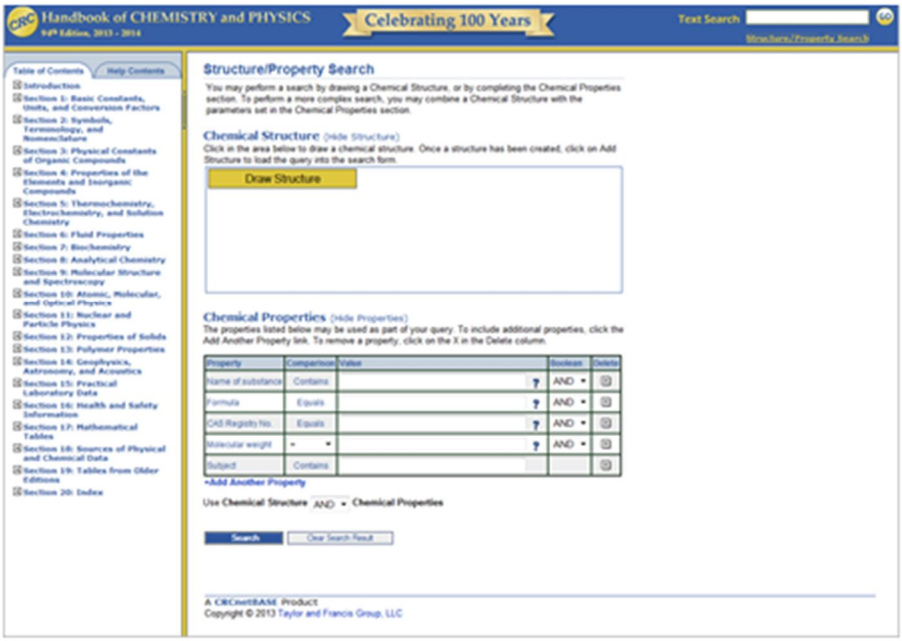
Combined Chemical Dictionary

An online database containing information on over 500,000 substances from the well-known printed Dictionaries of Organic Compounds, Inorganic and Organometallic Compounds, Analytical Reagents, Carbohydrates, Drugs and Natural Products. Search by name, formula, CAS Registry number or structure. It includes melting and boiling points, density, refractive index and journal references to synthesis and spectra.



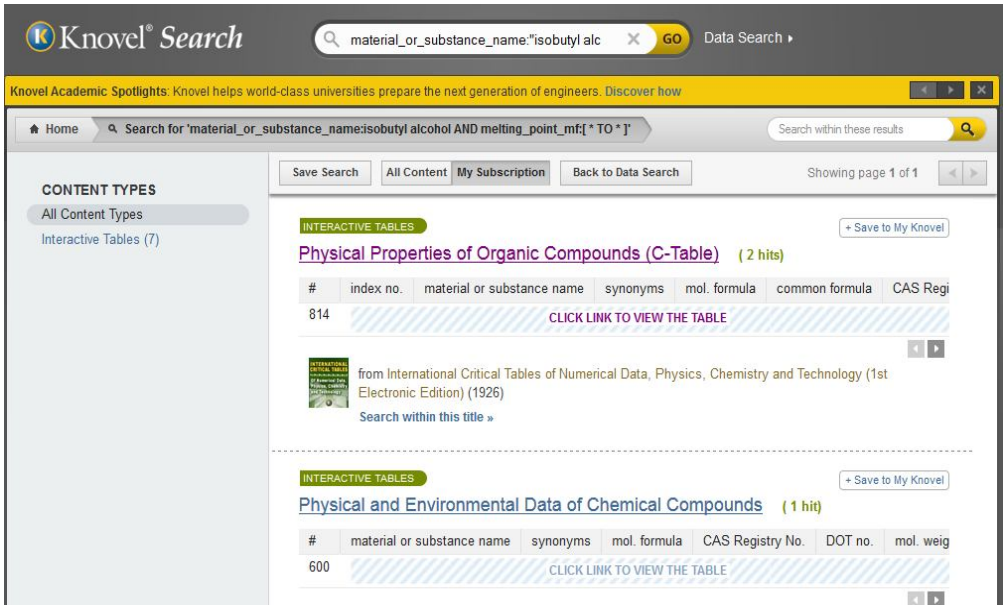
CRC Handbook of Chemistry and Physics

Contains information on approximately 11,000 substances, including melting point, boiling point, density, solubility and refractive index. It's available in print and online, but is not the easiest source to search. When using the print version, look up at the *property* in the index: for organic compounds you will find a table called 'Physical constants of organic compounds' which lists the substances alphabetically. When using the online version, use the *structure/property* search and enter a name, formula or CAS registry number or draw your compound. In the results, look for a link to an *interactive table.*



Knovel Library

This enables you to search across a range of different reference books including *DIPPR*, *Knovel Critical Tables* and *Yaws' Handbook of Physical Properties for Hydrocarbons and Chemicals*. Use the 'data search' link next to the main search box. Data is often provided in a table which may allow you to plot a graph, where appropriate. Don't reference the Knovel Library: write down the details of the specific book that the data comes from.



NIST Chemistry WebBook

Free, open access resource made available by the National Institute of Standards and Technology (USA). Search by compound name, CAS registry number, molecular formula or structure. The Chemistry WebBook is particularly useful for thermochemical data for both vapour and liquid phases, including enthalpy/entropy of formation, sublimation and fusion. Also provides Henry's Law data and ionisation energies. Melting and boiling points are available under 'phase change data': boiling point is labelled T_{boil} and melting point is labelled T_{fus}.

Condensed phase thermochemistry data

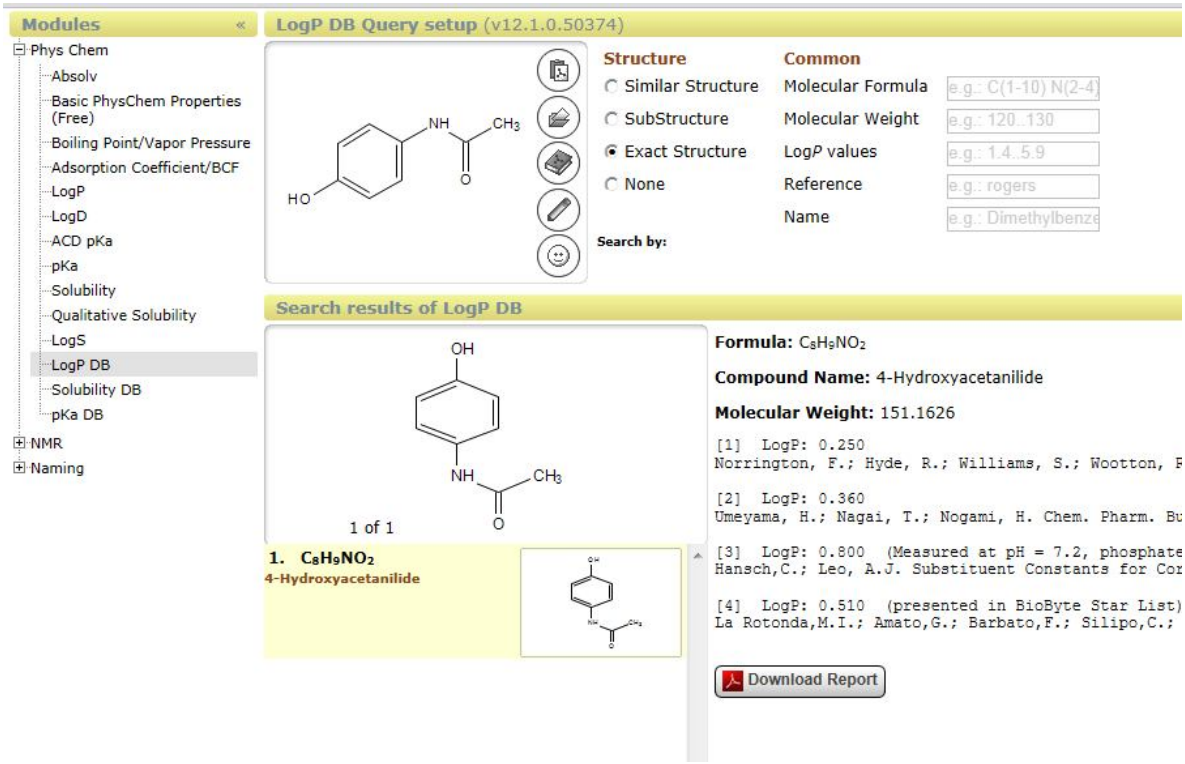
Go To: Top, References, Notes / Error Report

Data compiled as indicated in comments:
ALS - H.Y. Afeefy, J.F. Liebman, and S.E. Stein
DH - E.S. Domalski and E.D. Hearing

Quantity	Value	Units	Method	Reference	Comment
$\Delta_f H°_{solid}$	-165.0	kJ/mol	Ccb	Cox, 1961	*ALS*
$\Delta_f H°_{solid}$	-165.1 ± 1.3	kJ/mol	Ccb	Andon, Biddiscombe, et al., 1960	*ALS*
$\Delta_f H°_{solid}$	-162.8 ± 1.0	kJ/mol	Ccb	Parks, Manchester, et al., 1954	*ALS*
$\Delta_f H°_{solid}$	-163.9	kJ/mol	Ccb	Badoche, 1941	Author's hf298_condensed=-41.49 kcal/mol; *ALS*
Quantity	**Value**	**Units**	**Method**	**Reference**	**Comment**
$\Delta_c H°_{solid}$	-3058. ± 10.	kJ/mol	AVG	N/A	Average of 6 values; Individual data points
Quantity	**Value**	**Units**	**Method**	**Reference**	**Comment**
$S°_{solid,1\ bar}$	144.01	J/mol*K	N/A	Andon, Counsell, et al., 1963	*DH*
$S°_{solid,1\ bar}$	142.7	J/mol*K	N/A	Parks, Huffman, et al., 1933	Extrapolation below 90 K, 49.04 J/mol*K.; *DH*

ACD/i-Lab

Available via RSC National Chemical Database Service. This is primarily a tool for predicting properties but contains literature values for logP, solubility and pKa. Look for a link in the left hand menu that says 'DB'. DB means 'database' and gives experimental values.



Detherm

Available via RSC National Chemical Database Service. Detherm gives thermophysical properties of pure substances **and mixtures** including vapour pressure, viscosity and phase equilibria.

SciFinder and Reaxys

These large literature databases provide property data for millions of compounds. They are best used to find data for compounds that are rarely reported in the literature: you will get too many values for common compounds and the values will vary considerably making it difficult to choose the 'correct' value. Property data is mainly derived from the journals and patents indexed by the databases: it is advisable to read the original article to view the conditions under which the data was obtained. SciFinder has additional data from a number of sources including graphical spectra from Wiley and AIST and predicted property values from ACDLabs.

For help with finding physical and chemical property data, please contact your subject librarian.

LJH May 2014