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The LOGKow Database

A Comprehensive Compilation of Octanol/Water Partition Coefficients (LogP)

The LOGKOW Database is a valuable resource with many applications such as Extraction Procedures, Chemical Regulatory Compliance, Pharmaceutical R&D, Pesticide Design, Environmental Hazard Assessment for and processes where the Biological Activity of Chemicals is modeled.

The LOGKow is the equilibrium ratio of solute concentrations in two immiscible solvents; it describes how much of a given solute dissolves in octanol versus the amount which dissolves in water. This ratio is closely related to a chemical's ability to be absorbed and transported within a biological system. The LOGKow is a critical parameter in the evaluation of new drugs, environmental risk assessment, and chemical safety assessment, classification and labeling.

The **LOGKOW Database** is maintained and updated by Dr James Sangster, an internationally recognized authority in the field. The compilation includes:

- **over 38,000 evaluated octanol/water partition coefficients for over 24,000 organic compounds**
- **over 12,000 'recommended' partition coefficient values.**
- **approximately 3,000 current literature references in Chemical Abstracts style.**
- **the acid dissociation constants (pKa).**
- **Information about the method of measurement** *:*
  - ***direct method*** - the pH, temperature, phases analyzed, nature of the aqueous phase, method and method reference are given (e.g. “Shake Flask RC pH7.4 in Water”)
  - ***indirect method*** - a short description of the method is given (e.g. “HPLC retention time correlation”)
- **Chemical Identifiers: the CAS Registry Number, SMILES notation and molecular formula.**

Important LOGKow Applications

A LOGKow value can provide environmental scientists with an indication of how easily a compound might be taken up in groundwater or pollute waterways and, its toxicity to terrestrial animals and aquatic life. In medicine, pharmacology and drug design, the LOGKow is an important indicator of the ADME activity (Absorption, Distribution, Metabolism and Excretion) of a substance. However, a LOGKOW value is only as reliable as the accuracy of its measurement. LOGKOW values in the compilation are of the highest quality and accuracy available. In fact, The European Chemical Agency in their REACH guidelines explicitly state that for regulatory compliance reporting "experimentally derived high-quality Kow values or values which are evaluated in reviews and assigned *recommended values* are preferred over other determinations of Kow." One of Dr. Sangster's publications (1989)[1] is cited in the guidelines as a key reference.

Medicinal Chemists and Pharmacologists who are active in drug design and Environmental Engineers, Analytical Chemists and Toxicologists involved in environmental impact analyses; risk assessment; the prediction of bioconcentration in soil and water, the absorption of organic pollutants; and, the solubility and modeling of the environmental fate of organic chemicals find the log Kow essential to their work.

The **LOGKOW Database** is available as flat files and in a spreadsheet format.

[1]Sangster, J. (1989) "Octanol-water partition Coefficients of Simple Organic Compounds." In ECHA REACh Guidelines, Chapter R.7A Section (R.7.1.8.4) Conclusions on Partition Coefficient n-Octanol/Water.

For more information, please contact:

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