



LOGKOW Factsheet

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The LogKow Database

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

The LogKow Database is a valuable compilation of octanol-water partition coefficients and related data with many important applications involving: extraction procedures, chemical regulatory compliance, pharmaceutical R&D, pesticide design, and environmental hazard assessment and extraction procedures.

The LogKow is the equilibrium ratio of solute concentrations in octanol and water, two immiscible solvents; it measures how much 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. It is a critical parameter in the evaluation of new drugs, environmental risk assessment, chemical safety assessment, classification and labeling. The Database includes:

- 28,726 unique chemicals (carbon number range C1 - C254)
- 44,800 evaluated octanol/water partition coefficients
- 12,765 recommended partition coefficient values
- 3,879 references in Chemical Abstracts style.
- 3,925 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 shorter description of the method is given (e.g. "HPLC retention time correlation")
- chemical Identifiers: over 90% of LogKow chemicals are identified by CAS Registry Numbers and SMILES notations and a molecular formula.
- The LogKow Database is available in the following formats: tab-delimited text records, Excel format and in MySQL dumpfile format.



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Important LogKow Applications

LogKow values 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.

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 the bioconcentration in soil and water, the absorption of organic pollutants and, modeling the environmental fate of organic chemicals find the LogKow essential to their work.

The LogKow Database is maintained and updated regularly by Dr. James Sangster, an internationally recognized authority in the field. A LogKow value is only as reliable as the accuracy of its measurement and publications included in the Database are of high quality and accuracy. The European Chemical Agency (ECHA) in their REACH guidelines states 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 has been cited in the guidelines as a key reference.



¹Sangster, 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](#).

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