LOGKOW
A Databank of Evaluated Octanol-Water Partition Coefficients
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ABSTRACT

The octanol-water partition coefficient is a laboratory-measured property of a
substance. Partition coefficients are used extensively in medicinal chemistry, drug design,
ecotoxicology and environmental chemistry. A very large compilation of partition
coefficients is described, which contains also details of experimental measurement, CAS
Registry Numbers, Recommended Values and literature references in Chemical Abstracts
form.

Introduction

If a third substance be added to two immiscible solvents in contact, it will distribute
itself between the two solvents. At equilibrium, the ratio of solute concentrations in the two
solvents will attain a definite value. This was noticed at an early date (1).

The value of this partition coefficient will in general depend upon temperature,
pressure, concentration and the nature of solvents and solute. As used in the present context,
the partition coefficient usually refers to very dilute solutions, in which the solute has the
same molecular form in both solvents. (Thus organic acids – which dimerize – and salts –
which ionize – are usually excluded from this strict definition).

The octanol-water partition coefficient, $K_{\text{ow}}$, is a thermodynamic measure of the
tendency of a solute to prefer a non-aqueous milieu to water. The octanol-water pair has been
of particular interest for at least 30 years (2). It was known, from about 1900, that the narcotic
action of many organic compounds could be correlated with their oil-water partition
coefficients. In modern times, the “oil” of preference has become octanol (3).

Currently, $K_{\text{ow}}$ has wide use in two principal areas, viz., medicinal chemistry/drug
design and environmental chemistry. In medicinal chemistry, its usefulness resides in its
participation in quantitative structure-activity relationships (often abbreviated as QSAR). A
QSAR may take the form

$$BR = a + b \log K_{\text{ow}}$$

where $BR$ is biological response (protein-ligand binding, metabolism, CNS agent and
microbial action, etc.)(4). In environmental chemistry, the general relation (1) has been useful
in correlating such properties of organic pollutants as bioaccumulation and soil-water
partition coefficients (5,6).
Data Evaluation in the Databank

Like any physico-chemical property, $K_{ow}$ may be measured in a number of ways. The methods differ enormously in ease of execution, inherent precision, apparatus required, etc. (7). For example, the reported $K_{ow}$ data for DDT cover a range of 1000 (8). The author has compiled a Databank of experimental $K_{ow}$ data for over 20,000 compounds (8). In addition to the $K_{ow}$ data themselves, details of experimental measurement, abstracted from original publications are also included, as well as Recommended Values (wherever possible). Data sources are fully referenced.

Search and display of data in LOGKOW

The Databank may be searched by molecular formula, by Chemical Abstracts Registry Number or in “browse” mode. A typical output data display for a compound is given in Fig. 1. In addition to the data already mentioned, the display includes IUPAC names, $pK_a$ values and S.M.I.L.E.S. notation (Simplified Molecular Input Line Entry System: a method for representing the structure of a molecule as a string of ASCII symbols).

Availability and Updating

The Databank is available online at www.tds-tds.com. A version on PC diskettes may be purchased from the author. It is hoped that the Databank will be available free of charge on the Internet in future.

The Databank is updated monthly.

REFERENCES

**Figure 1**

**FORMULA:** $C_7H_6O_3$  
**CAS#:** 99-06-9  
**pKₐ:** 4.05  

**NAME:** Benzoic acid, 3-hydroxy-  

**SMILES:** `c1c(O)cc(C(=O)O)cc1`

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Footnote:  
53: filter-probe rapid-mix apparatus  
59: ion-corrected to neutral form

**RECOMMENDED VALUE:** 1.50

**References:**


Etc.