

IUPAC Wire

for nominating me and also my many academic and industrial collaborators across the world, including various current and former scientists at DSM. As a polymer chemist, I believe that the most interesting problems are best identified by working across academic disciplines, often in close partnership with industrial colleagues."

Dr. Marcel Wubbolts stated that "The jury recognizes the broad impact of Professor Armes' work, as is also exemplified by statements of experts in the field of Polymer Chemistry. The theme of this year's Award was Macromolecular Architecture for Brighter Living, and Prof. Armes' work resonates with all aspects of this theme. Professor Armes has also been actively involved in turning academic knowledge into societally relevant solutions to needs. I'm really looking forward to seeing the progress he will make during the rest of his career."

DSM bestows the Materials Sciences Award every two years in recognition of outstanding scientific work by an established scientist who has contributed significantly to the advancement of the Materials Sciences field. The Award forms part of DSM's Bright Science



(from left to right) Marcel Wubbolts, Steve Armes, and Rolf Benthem-van.

Awards Program, and is designed to recognize and reward lifetime achievement on the part of seasoned scientists from all over the world. Previous recipients include Professor Jiang Ping Gong of the Faculty of Advanced Life Science at Hokkaido University in Japan and Professor Geoff Coates of Cornell University (USA).

www.iupac.org/dsm-materials-sciences-award-2016

WANTED:

A Home for an Orphaned Chemical Database

LOGKOW—a databank of evaluated octanol-water partition coefficients

The octanol-water partition coefficient ($\text{Log } K_{\text{ow}}$, $\text{Log } P$) is a laboratory-measured property of a pure substance (gas, liquid or solid). Its importance for chemists is comparable to that of vapour pressure, solubility, Henry's law constant, melting and boiling points, etc. In particular, partition coefficients have been used extensively:

- in the design of new drugs and pharmaceuticals
- as a key parameter for modeling the fate of organic pollutants in soil, natural waters and the atmosphere
- as a quantitative measure of the hydrophilic/lipophilic balance of an organic compound
- in investigation of quantitative structure-activity relationships (QSAR) of organic compounds

The database was created in 1987 and has been continuously updated ever since. Currently it contains experimental data on about 29,000 organic and organometallic compounds. LOGKOW contains no calculated or estimated data.

Each compound is identified by molecular formula, IUPAC name, and Chemical Abstracts Registry Number. A pK_a value is given, where appropriate. Also included

is a S.M.I.L.E.S. string of characters which represents the three-dimensional structure (connectivity) of the molecule. For every numerical $\text{Log } K_{\text{ow}}$ datum, a literature source reference is given, in Chemical Abstracts style. Also, experimental conditions of measurement are noted (temperature, equilibration method, analytical method, nature of the aqueous phase, and which phases were analyzed). If the original data source reference gave a reference describing the experimental method, this secondary reference was included. Where warranted, a Recommended $\text{Log } K_{\text{ow}}$ value is indicated. The database can be searched by the molecular formula or Registry Number of the compound of interest.

The database, as a Java application, was hosted for 10 years by the National Research Council of Canada (Ottawa), with free access available via the Internet. The database, although it still exists, is no longer generally available for the use of chemists. The present communication is a call for an appropriate institution to restore LOGKOW to its rightful place on the Internet.

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