



Standard Test Method for Partition Coefficient (N-Octanol/Water) Estimation by Liquid Chromatography¹

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1. Scope

1.1 This test method describes a procedure for the estimation of the log of the octanol/water partition coefficient ($\log K_{ow}$) of chemicals over the range from 0 to 8.

1.2 This test method uses an empirically derived equation to relate the octanol/water partition coefficient to an experimentally determined retention time on a liquid chromatographic column.

1.3 This test method has been designed to estimate $\log K_{ow}$ values for both non-ionizable and ionizable compounds. This is accomplished by buffering the liquid chromatographic solvent at a pH that will force the test compound into either the non-ionized or ionized form.

1.4 This test method requires some knowledge of the detector response to the chemical being tested.

1.5 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish safety and health practices and determine the applicability of regulatory limitations prior to use.*

2. Referenced Documents

2.1 ASTM Standards:

D 1193 Specification for Reagent Water²

E 200 Practice for Preparation, Standardization, and Storage of Standard Solutions for Chemical Analysis³

E 682 Practice for Liquid Chromatography Terms and Relationships⁴

E 1022 Practice for Conducting Bioconcentration Tests with Fishes and Saltwater Bivalve Molluscs⁵

3. Terminology

3.1 Definitions:

3.1.1 *octanol/water partition coefficient (K_{ow})*—the equilibrium ratio of the molar concentrations of a chemical in

n-octanol and water, in dilute solution. K_{ow} is a constant for a specific chemical at a given temperature. Since K_{ow} is the ratio of two molar concentrations, it is a dimensionless quantity. K_{ow} is often reported as $\log K_{ow}$.

3.1.2 *retention time (t_R , t_o)*—the reference compound or test chemical retention time (t_R) is the time from sample injection to maximum concentration (peak height) of eluted reference compound or test chemical. The internal standard retention time (t_o) is the time from sample injection to the maximum concentration (peak height) of the eluted internal standard.

4. Summary of Test Method

4.1 This test method is based on the work of Veith et al (1).⁶ Another similar test method is available from OECD (2).

4.2 The test substance (solute) is injected onto a liquid chromatograph column containing a solid-phase support onto which a commercially available long-chain hydrocarbon (for example C8 or C18) has been bonded. Chemicals injected onto such a column move along it by partitioning between the mobile phase and the stationary hydrocarbon phase. A methanol/water solvent system is typically used to elute the solute which is subsequently analyzed using an ultraviolet/visible absorption detector, refractive index detector, electrochemical detector, or other appropriate detector. If the test substance is not amenable to detection by the available LC detectors, the analyst may collect fractions of the column effluent and analyze for the test substance using gas chromatography, liquid scintillation, or other appropriate technique.

4.3 The K_{ow} of the test compound is estimated from a linear regression equation developed from a plot of $\log(t_R - t_o)$ versus $\log K_{ow}$, using data determined in a calibration step that involves injecting into the chromatograph a mixture of reference chemicals.

4.4 A calibration graph of $\log(t_R - t_o)$ versus $\log K_{ow}$ is developed for a number of reference compounds (typically between 5 and 10) which are structurally similar to the test chemical. Lists of values of measured $\log K_{ow}$ are available for many chemicals (3, 4, 5). If data on the partition coefficients of structurally related compounds are not available, a more general calibration graph must be developed using other reference compounds. This is a less accurate approach than that

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² Annual Book of ASTM Standards, Vol 11.01.

³ Annual Book of ASTM Standards, Vol 15.05.

⁴ Annual Book of ASTM Standards, Vol 14.01.

⁵ Annual Book of ASTM Standards, Vol 11.05.

⁶ The boldface numbers in parentheses refer to the list of references at the end of this test method.