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## 40 C.F.R. § 799.6755

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### TSCA partition coefficient (n-octanol/water), shake flask method.

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(a) *Scope—(1) Applicability.* This section is intended to meet the testing requirements of the Toxic Substances Control Act (TSCA) (15 U.S.C. 2601).

(2) *Source.* The source material used in developing this TSCA test guideline is the Office of Prevention, Pesticides and Toxics (OPPTS) harmonized test guideline 830.7550 (August 1996, final guideline). The source is available at the address in paragraph (f) of this section.

(b) *Introductory information—(1) Prerequisites.* Suitable analytical method, dissociation constant, water solubility, and hydrolysis (preliminary test).

(2) *Coefficient of variation.* The coefficient of variation on the mean values reported by the participants of the Organization for Economic Cooperation and Development (OECD) Laboratory Intercomparison Testing, Part I, 1979, appeared to be dependent on the chemicals tested; it ranges from 0.17 to 1.03.

(3) *Qualifying statements.* This method applies only to pure, water soluble substances which do not dissociate or associate, and which are not surface active. In order to use the partition coefficient (P) as a screening test for bioaccumulation, it should be ascertained that the impurities in the commercial product are of minor importance. Testing of P (n-octanol/water) cannot be used as a screening test in the case of organometallic compounds.

(4) *Alternative methods.* High-pressure liquid chromatography (HPLC) methods described in the references in paragraphs (f)(3), (f)(4), and (f)(5) of this section may be considered as an alternative test method.

(c) *Method—(1) Introduction, purpose, scope, relevance, application, and limits of test.* The P of a substance between water and a lipophilic solvent (n-octanol) is one model variable which may be used to describe the transfer of a substance from the aquatic environment into an organism and the potential bioaccumulation of the substance. Studies show a highly significant relationship between the P of different substances in the system water/n-octanol and their bioaccumulation in fish described in paragraph (f)(1) of this section.

(2) *Definitions—Partition coefficient (P)* is defined as the ratio of the equilibrium concentrations ( $C_i$ ) of a dissolved substance in a two-phase system consisting of two largely immiscible solvents. The P therefore is the quotient of two concentrations and is usually given in the form of its logarithm to base 10 ( $\log P$ ). In this case n-octanol and water:

Equation 1:

$$P_{ow} = C_{n\text{-octanol}} / C_{\text{water}}$$

(3) *Reference substances.* The reference substances need not be employed in all cases when investigating a new substance. They are provided primarily so that calibration of the method may be performed from time to time

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and to offer the chance to compare the results when another method is applied. The values presented in table 1 of this section are not necessarily representative of the results which can be obtained with this test method as they have been derived from an earlier version of the test guideline.

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