

Analytical Data Summary

PFOS, Primary Standard - Test Control Reference #TCR-00017-046

SOLUBILITY IN WATER, NATURAL SEAWATER, AN AQUEOUS SOLUTION OF 3.5% SODIUM CHLORIDE, AND N-OCTANOL WITH SUBSEQUENT CALCULATION OF THE N-OCTANOL:WATER PARTITION COEFFICIENT (K_{ow}) OF PFOS FOR EACH OF THE AQUEOUS MATRICES

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INTRODUCTION

Solubility is an environmentally significant parameter because the spatial and temporal movement (mobility) of a substance through the environment is largely determined by its solubility in water. Water-soluble substances gain ready access to humans and other living organisms. The knowledge of the solubility of a substance in water is a prerequisite for testing biological degradation and bioaccumulation in water and many other tests. Solubility data can also be used for comparative and modeling purposes.

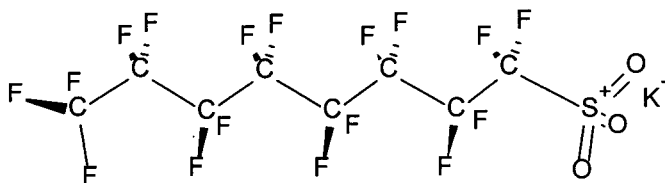
Another significant parameter, the n-octanol/water partition coefficient (K_{ow}), is defined as the ratio of the equilibrium concentrations of a dissolved substance in a two-phase system consisting of two largely immiscible solvents. The partition coefficient of a substance between water and a lipophilic solvent (n-octanol) is one model variable which may be used to describe both the transfer of a substance from the aquatic environment into an organism and the potential bioaccumulation of the substance. Studies have shown there is a highly significant relationship between the partition coefficient of different substances in the system n-octanol/water and their bioaccumulation in fish, as described by Neely, W.B., et al. "Partition Coefficients to Measure Bioconcentration Potential of Organic Chemicals in Fish"; Environmental Science and Technology 8:1113 (1975).

PURPOSE

The purpose of this analytical data summary is to combine the solubility data for PFOS (TCR-00017-046) in ASTM Type I water, natural seawater, an aqueous solution of 3.5% sodium chloride, and n-octanol into a single document. This data was previously reported in 3M Environmental Laboratory Reports #E00-1716 Phase: Solubility of PFOS in Water, #E00-1716 Phase: Solubility of PFOS in Natural Seawater and an Aqueous Solution of 3.5% Sodium Chloride, and #E00-1716 Phase: Solubility of PFOS in n-Octanol.

In addition, calculations were performed to determine the n-octanol:water partition coefficient (K_{ow}) for PFOS (TCR-00017-046) in each of the aqueous matrices. The calculated K_{ow} values are also presented in this document.

TEST SUBSTANCE



POTASSIUM PERFLUOROOCTANESULFONATE (PFOS)

#TCR-00017-046

Chemical Formula: $C_8F_{17}SO_3K$

CAS Number: 2795-39-3

Molecular Weight: 538.22 g/mol

PFOS, Test Control Reference #TCR-00017-046

Table 1. Characterization of the Test Substance and Analytical Reference Substance

TEST SUBSTANCE	PFOS	THPFOS
Source	Re-crystallized by George Moore, 3M Specialty Materials, Bldg. 236-1B-10	SynQuest Labs
Expiration Date	01-01-2010	Not Available
Storage Conditions	Frozen	Frozen
3M Laboratory Identification Number	TCR-00017-046	TCR-00017-047 Lot #Q75-30
Physical Description	White Powder	White Powder
Purity	* 97.9%	•

**The purity of the PFOS used in 3M Environmental Laboratory Report #E00-1716 was determined to be 97.9%. The purity of THPFOS (currently being determined by Centre Analytical Laboratory) will not affect any analytical findings. The same lots/source of both compounds were used throughout the entire study.*

TEST SYSTEMS

Table 2. Description of Test Systems

TEST SYSTEM	ASTM TYPE I WATER	NATURAL SEAWATER	SODIUM CHLORIDE	N-OCTANOL
Source	Millipore System	Ocean Scientific International	EM Science	Aldrich
Expiration Date	NA	2005	2010	11/01/01
Storage Conditions	Ambient	Ambient	Ambient	Flammable Cabinet
3M Laboratory Identification Number	NA	TN-A: 4193	TN-A: 2458	TN-A: 4703
Purity/Grade	ASTM Type I	Salinity 35	ACS Grade	99%+ HPLC Grade

SUMMARY OF PFOS (TCR-00017-046) SOLUBILITY

The approximate solubility of PFOS (TCR-00017-046) was determined in each of the solvents by performing a solubility screen test, followed by a quantitative solubility determination via Shake Flask Method.

Results are presented in table 3:

Table 3. Solubility of PFOS TCR-00017-046

SOLVENT	PFOS SOLUBILITY (CORRECTED FOR PURITY)
ASTM Type I Water	680 µg/mL *
Natural Seawater	12.4 µg/mL **
Aqueous Solution of 3.5% Sodium Chloride	20.0 µg/mL **
n-Octanol	56.0 µg/mL ***

* As reported by 3M Environmental Laboratory Report #E00-1716 Phase: Solubility of PFOS in Water, ** Phase: Solubility of PFOS in Natural Seawater and an Aqueous Solution of 3.5% Sodium Chloride, and *** Phase: Solubility of PFOS in n-Octanol.

All solubility determinations of PFOS TCR-00017-046 were conducted at 22-25 °C.

DETERMINATION OF THE PARTITION COEFFICIENT (N-OCTANOL/WATER) OF PFOS (TCR-00017-046) FOR EACH OF THE AQUEOUS MATRICES

United States Environmental Protection Agency OPPTS 830.7550, "Partition Coefficient (n-Octanol/Water), Shake Flask Method" and OECD 107, "Partition Coefficient (n-octanol/water): Shake Flask Method" guidelines define partition coefficient (K) as the ratio of the equilibrium concentrations of a dissolved substance in a two-phase system consisting of two largely immiscible solvents. In the case of n-octanol and water,

$$K_{ow} = C_{n-octanol} / C_{water}$$

The partition coefficient (K) is the dimensionless quotient of two concentrations, and is usually expressed as its logarithm to base 10.

OPPTS and OECD guidelines for the determination of partition coefficient (n-octanol/water) by shake flask method state the method is not applicable to strong acids and bases, metal complexes, substances which react with the solvent, or surface-active agents. Measurements should be made on ionizable substances in their non-ionized form (free acid or free base) only by using an appropriate buffer with a pH below the pK for a free acid or above the pK for a free base.

The physical properties of PFOS do not allow one to determine the partition coefficient by the shake flask method. However, individual solubility determinations of PFOS in water, natural seawater, an aqueous solution of 3.5% sodium chloride, and n-octanol have been conducted. The partition coefficient (n-octanol/water) was determined mathematically for each of the aqueous matrices. Results are summarized in Table 4.

Table 4. Calculated log K_{OW} for PFOS (TCR-00017-046) in Various Aqueous Matrices

AQUEOUS MATRIX	PFOS SOLUBILITY	CALCULATED LOG K _{OW}
ASTM Type I Water	680 µg/mL	-1.08
Natural Seawater	12.4 µg/mL	0.65
Aqueous Solution of 3.5% Sodium Chloride	20.0 µg/mL	0.45

METHOD SUMMARIES

The solubility determination of PFOS (TCR-00017-046) in each of the solvents was performed according to United States Environmental Protection Agency OPPTS 830.7840, "Water Solubility: Column Elution Method; Shake Flask Method" and OECD 105, "Water Solubility" Guidelines, using the 3M Environmental Laboratory methods ETS-8-170.0 "Solubility Screen Test: Approximate Solubility Determination of a Test Substance in Various Solvents;" and ETS-8-172.0 "Shake Flask Method; Solubility Determination of a Test Substance in Various Solvents". All analyses were performed according to the 3M Environmental Laboratory method ETS-8-155.0 "Analysis of Perfluorooctanesulfonate or Other Fluorochemicals in Waste Stream or Water Extracts Using HPLC-Electrospray/Mass Spectrometry".

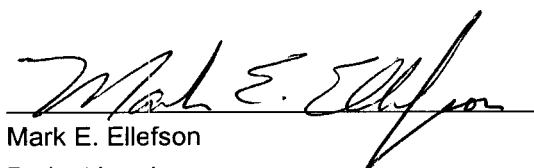
The n-octanol/water coefficient determinations of PFOS (TCR-00017-046) in each of the aqueous matrices were calculated according to United States Environmental Protection Agency OPPTS 830.7550 "Partition Coefficient (n-Octanol/Water), Shake Flask Method" and OECD 107, "Partition Coefficient (n-octanol/water): Shake Flask Method" Guidelines.

REFERENCES

1. Fate, Transport and Transformation Test Guidelines Office of Prevention, Pesticides and Toxic Substances (OPPTS) 830.7840 Water Solubility: Column Elution Method; Shake Flask Method. EPA 712-C-96-041, August 1996.
2. OECD 105: Water Solubility. Adopted 27 July, 1995.
3. Product Properties Test Guidelines Office of Prevention, Pesticides and Toxic substances (OPPTS) 830.7550 Partition Coefficient (n-Octanol/Water), Shake Flask Method, August 1996.
4. OECD 107: Partition Coefficient (n-octanol/water): Shake Flask Method.

SIGNATURE PAGE

We certify that this summary report is a true and complete representation of the data:



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05/09/01
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