OCTANOL/WATER PARTITION COEFFICIENT

TEST SUBSTANCE

Identity: Perfluorooctanoic acid, ammonium salt; may also be referred to as PFOA ammonium salt, Ammonium perfluorooctanoate, FC-116, FC-126, FC-169, or FC-143. (Octanoic acid, pentadecafluoro-, ammonium salt, CAS # 3825-26-1)

Remarks: The 3M production lot number was not recorded. The subject compound is FC-143. It's purity was not sufficiently characterized, though current information indicates it is a mixture of 96.5 - 100% test substance and 0 – 3.5% C_6, C_7, and C_9 perfluoro analogue compounds.

METHOD

Method: Calculation
GLP (Y/N): No
Year completed: 1981
Remarks: Manual calculation using a published method for determining partition coefficients based on chemical fragments / functional groups.

RESULTS

Calculated $\log P_{ow}$ for FC-143 = -0.9

CONCLUSIONS

This calculation indicates that ammonium perfluoroocanoate (FC-143) has an octanol / water partition coefficient of approximately 0.126.

Submitter: 3M Company, Environmental Laboratory, P.O. Box 33331, St. Paul, Minnesota, 55133

DATA QUALITY

Reliability: Klimisch ranking 2.

REFERENCES

Calculation done by the 3M Company, Dr. E.A. Reiner of the 3M Environmental Laboratory, St. Paul, MN, December 7, 1981.

OTHER

Last changed: 5/24/00

FC-143
Calculated log P

$CF_3 \cdot CF_2 \cdot CF_2 - CF_2 - CF_2 - CF_2 - CF_2 - \overset{O}{\overset{\|}{C}} - O^-$

$f_{-CO_2^-}$	1 (-5.19)		-5.19
f_C	7 (0.20)		+1.4
f_F	15 (-0.38)		-5.7
F_b	21 (-0.12)	7 C bonds + 15 C-F bonds = 22 = n. n-1 = 21	-2.52
$3\ F_{mhG_3}$	3 (0.53)		+1.59
$12\ F_{mhG_2}$	12 (0.30)		+3.6
$14\ F_{mhV_{15}}$	14 (0.28)	n=15, n-1=14	+3.92
F_{H/SP_2}	(2 F α to COO^-) No values are tabulated for COOH and F. By analogy with COOH and Cl, a value of ~2 would be expected from the 2 α F. ∴ assume 2		+2.0
Calculated log P for FC-143			-0.9

Ref: Chapter IV, The Fragment Method of Calculating Partition Coefficients, Substituent Constants for Correlation Analysis in Chemistry and Biology by Corwin Hansch and Albert Leo (1979) John Wiley and Sons, Inc.

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