

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% C₆, C₇, and C₉ 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 logP_{ow} for FC-143 = -0.9

CONCLUSIONS

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

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DATA QUALITY

Reliability: Klimisch ranking 2.

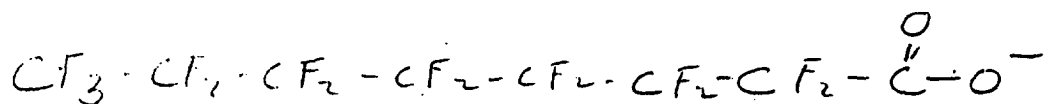
REFERENCES

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



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 CF bonds 22 = n n-1=21	-2.52
3 F _{mh} G ₃	3 (0.53)	+1.59
12 F _{mh} G ₂	12 (0.30)	+3.6
14 F _{mh} V ₁₅	14 (0.28) n=15, n-1=14	+3.92
F _{H/SP₂} (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.

EAK 12-7-81