

## 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<sub>6</sub>, C<sub>7</sub>, and C<sub>9</sub> 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<sub>ow</sub> for FC-143 = -0.9

CONCLUSIONS

This calculation indicates that ammonium perfluorooctanoate (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

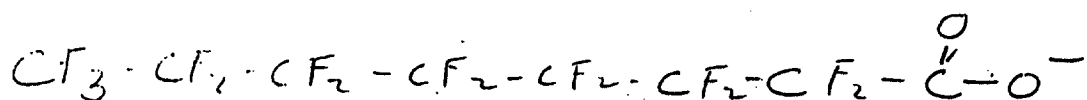
Calculation done by the 3M Company, Dr. E.A. Reiner of the 3M Environmental Laboratory, St. Paul, MN, December 7, 1981.

OTHER

**Last changed:** 5/24/00

FC-143

Calculated log P



|                                                            |                                                                                                                                 |       |
|------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------|-------|
| f - CO <sub>2</sub> <sup>-</sup>                           | 1 (-5.19)                                                                                                                       | -5.19 |
| f C                                                        | 7 (0.20)                                                                                                                        | +1.4  |
| f F                                                        | 15 (-0.38)                                                                                                                      | -5.7  |
| F <sub>b</sub>                                             | 21 (-0.12) 7 C bonds<br>+ 15 CF bonds<br>22 = n. n-1 = 21                                                                       | -2.52 |
| 3 F <sub>mh</sub> G <sub>3</sub>                           | 3 (0.53)                                                                                                                        | +1.59 |
| 12 F <sub>mh</sub> G <sub>2</sub>                          | 12 (0.30)                                                                                                                       | +3.6  |
| 14 F <sub>mh</sub> V <sub>15</sub>                         | 14 (0.28) n=15, n-1=14                                                                                                          | +3.92 |
| F <sub>H/SP<sub>2</sub></sub> (2 F α to COO <sup>-</sup> ) | No values are tabulated for COOH and F. By analogy with COOH and Cl, a value of ~2 would be expected from the 2nd 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

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