

BIOCONCENTRATION (n-OCTANOL/WATER PARTITION COEFFICIENT)

TEST SUBSTANCE

Identity: N-methylperfluorooctane sulfonamidoethanol; may also be referred to as N-MeFOSE Alcohol, FC-790, FM-3925 or T-5874. (1-Octanesulfonamide, N-methyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-N-(2-hydroxyethyl)-, CAS # 24448-09-7)

Remarks: Material is a cream-colored solid of uncharacterized purity Batch 2334.

METHOD

Method/guideline followed: Based on OECD 117 and EEC-Directive 92/69 EEC, Annex V, Part A.

Type: Partition coefficient (n-octanol/water)

GLP (Y/N): Yes

Year: 1994

Test Temperature: 20.2-20.6°C (mobile phase)

Analytical: High Performance Liquid Chromatography with spectrophotometric detector. Stationary phase was bonded silica C₁₈. Mobile phase was 75/25 (v/v) acetonitrile/water

Remarks: The sample was indicated to be 100% pure, but no analytical data is presented to confirm this claim.

The logP value was calculated from the chromatographic retention data, utilizing the capacity factor (k') as a proportional value to the partition coefficient. The capacity factor was calculated from the retention of the substance concerned (t_r) and the unretarded component (t₀):

$$k' = (t_r - t_0)/t_0$$

Using the results of reference substances, a plot of logP (x-value) versus log k' (y-value) was constructed, using linear regression analysis.

RESULTS

Substance	T_r ¹	K'	log k'	log P_{ow}	P_{ow}
Benzyl alcohol	1.14	0.274	-0.563	1.1	Not calculated
Toluene	2.24	1.503	0.177	2.7	Not calculated
1,4-dichlorobenzene	2.89	2.229	0.348	3.4	Not calculated
Fluoranthene	5.67	5.330	0.727	4.7	Not calculated
Dibenzyl	4.07	3.547	0.550	4.8	Not calculated
2,4-DDT	9.12	9.190	0.963	6.2	Not calculated
					Not calculated
Test substance					
Peak 1	7.70	7.598	0.881	5.6 ²	39.8 x 10 ⁴
Peak 2 (major component)	4.05	3.525	0.547	4.4 ²	2.51 x 10 ⁴
Several small peaks	1.6/4	0.79/3.47	-0.10/ 0.54	2.2/ 4.4 ²	1.50 x 10 ² / 2.52 x 10 ⁴

1. Mean value of the retention times of both chromatograms.

2. Interpolated from the regression line: $y = 0.288x - 0.730$ ($r=0.972$, $n=6$)

Note: The calculations were performed using values that were not rounded.

CONCLUSIONS

This data indicates that N-MeFOSE alcohol has a log octanol/water partition coefficient (logP) of 4.4, calculated using the peak considered to be the major component (Peak 2).

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

DATA QUALITY

Reliability: Klimisch ranking 2. This study meets most of the criteria for quality testing. The sample purity was not properly characterized.

REFERENCES

This study was conducted by NOTOX B.V., Hambakenwetering 3, 5231 DD 's-Hertogenbosch, The Netherlands at the request of 3M, Belgium. NOTOX Project 121275, "DETERMINATION OF THE PARTITION COEFFICIENT (N-OCTANOL/WATER) OF T-5874 BY HIGH PERFORMANCE LIQUID CHROMATOGRAPHY (HPLC)", April 07, 1994 .

OTHER

Last changed: 6/27/01

