ORIGINAL

AR226-0972

BIOCONCENTRATION (DISTRIBUTION COEFFICIENT)

TEST SUBSTANCE 8EHQ-0800-373

Identity: N-methylperfluorooctane sulfonamidoethanol; may also be referred to as N-MeFOSE Alcohol, FC-790, or FM-3925. (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 an off-white, waxy solid of uncharacterized purity.

METHOD

Method/guideline followed: 3M Environmental Laboratory protocol
Type: n-Octanol/Water distribution
GLP (Y/N): No
Year: 1979
Test Temperature: ~22°C

Remarks field: Testing was done on 3M Production lot 505. The sample was used "as received" without characterization of purity.

Two concentrations of N-MeFOSE alcohol in n-octanol were prepared; One at 1000 mg/L and one at 2000 mg/L. High concentrations were used to compensate for a lack in analytical procedures sufficiently sensitive to detect the N-MeFOSE alcohol in the sample re-extracted from the water phase into ethyl acetate.

25 mL of each solution were added to amber glass jars, each containing 900 mL of deionized water. They were shaken for approximately 16 hours at which point the octanol phase was drawn off and the water phase was placed in 250 mL polycarbonate centrifuge tubes and centrifuged at 13,700xG for 15 minutes. Water-phase aliquots from each were then transferred by pipet through two separatory funnels to insure removal of any octanol contamination. The samples were then extracted three times with ethyl acetate, concentrated, and analyzed by electron capture gas chromatography.

RESULTS

Concentration in the water phases shaken with 1000 ppm and 2000 ppm N-MeFOSE alcohol / n-octanol solutions were 0.0189 ppm and 0.033 ppm respectively.

n-Octanol/Water Distribution Coefficient:
1000 ppm test solution: 52,900

2000 ppm test solution:	60,600
Average:	56,800

CONCLUSIONS

This data indicates that N-MeFOSE alcohol has the potential to bioconcentrate in living organisms.

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

DATA QUALITY

Reliability: Klimisch ranking 3. While this study met with the standards at the time, the data is not reliable. Test substance lot 505 purity was not properly characterized. Validity of the analytical method was not evaluated, hence, the limit of detection / limit of quantitation, reproducibility, etc. are unknown. Because the solubility of the test substance in n-octanol is not known, the concentration of the test n-octanol solutions may exceed this limit. No attempt was made to analyze the n-octanol phase for the test substance. It is better practice to analyze both the octanol and water phases. This was done in previous attempts to measure octanol/water partition coefficients at lower octanol concentrations and the N-MeFOSE alcohol concentration was not measurably lower in the octanol phase. The procedure itself lacked the ability to compensate for potential losses of the material through sorption onto transferring vessels (e.g., the pipet and separatory funnels). A characteristic which is now understood. Calculation error in reported n-octanol/water distribution coefficient. Result should read 56,750 instead of 56,800. Another significant limitation of this study is that it used nonspecific analytical techniques. Additionally, there are at least 3 major components in N-MeFOSE alcohol. Octanol/water partition coefficients should be measured on pure compounds.

REFERENCES

3M Technical Report "Distribution Coefficient of FM 3925 in n-Octanol/Water." E. A. Reiner, Project 9970012600, Premanufacturing Notice FC-790, Report Number 015, January 10, 1979

OTHER

Last changed: 5/17/00

3M COMPANY
Form 6747-11-A

TECHNICAL REPORT SUMMARY

Date: 1/10/79

TO: TECHNICAL COMMUNICATIONS CENTER – 201-2CN

(Important – If report is printed on both sides of paper, send two copies to TCC.)

Division: Environmental Laboratory (EE & PC)	Dept. Number: 0535
Project: Premanufacturing Notice FC-790	Project Number: 9970012600
Report Title: Distribution Coefficient of FM 3925 in n-Octanol/Water	Report Number: 015
To: V. Pothapragada	
Author(s): E. A. Reiner	Employee Number(s): 47816
Notebook Reference: 48838, pp. 6, 8, and 9.	No. of Pages Including Coversheet:

SECURITY ▶ ☒ Open (Company Confidential) ☐ Closed (Special Authorization)

3M CHEMICAL REGISTRY ▶ New Chemicals Reported ☐ Yes ☒ No

KEYWORDS: (Select terms from 3M Thesaurus. Suggest other applicable terms.)

Distribution Coefficient

Partition Coefficient

Bioconcentration

Fluorochemical

CURRENT OBJECTIVE:

To determine the distribution coefficient of FM 3925 between n-octanol and water.

REPORT ABSTRACT: (200-250 words) This abstract information is distributed by the Technical Communications Center to alert 3M'ers to Company R&D. It is Company confidential material.

The distribution coefficient of FM 3925, lot 505, between n-octanol and water was measured according to a modification of the Environmental Laboratory procedure. The distribution coefficient was determined to be 56,800. This result suggests that this material is likely to accumulate in aquatic organisms to levels above the ambient aquatic concentration.

006535

Information Liaison Initials: SLW

Introduction

Living organisms possess the ability to concentrate and accumulate lipophilic organic compounds either directly from their environment or from their food source, a phenomenon which is well document (1,2).

In 1975 Neely, et al (3), demonstrated that the partition coefficient can be used to estimate this bioconcentration potential. As a result, it has become a common procedure to estimate bioconcentration potential from a compound's partition or distribution coefficient.

Methods

The distribution coefficient of FM 3925, lot 505, was determined by a modification of the 3M Environmental Laboratory protocol. The modifications and unique features of this study are described below.

FM 3925, lot 505, was used in the distribution coefficient determination as it was received without any further purification. Gas chromatographic analysis of this compound shows that this compound elutes as three overlapping peaks (Figure 1). The combined area of these peaks was used in the determination of sample concentrations.

Sample analysis was performed on a Hewlet-Packard Model 5713 gas chromatograph, a ^{63}Ni electron capture detector. Separations were obtained using a 6 ft. by 1/8 in. O.D. stainless steel column containing 10% Carbowax 20M on 60/80 mesh Chromosorb W-AW. Injection port, oven and detector temperatures were set at 200°, 180°, and 300° C., respectively. The gas flow rate was 40 ml/min. of a 95% Argon 5% methane mixture.

Two 25-ml n-octanol solutions of FM 3925 were added to amber glass jars, each containing 900 ml of deionized water. These n-octanol solutions contained 1000 ppm (0.018M) and 2000 ppm (0.036M) of FM 3925. High FM 3925 concentrations were used because earlier attempts at determining the distribution coefficient with concentrations below 0.01M were unsuccessful since our analytical procedures were not sufficiently sensitive to detect the FM 3925 re-extracted from the water phase into ethyl acetate.

The jars used in the distribution coefficient determination were shaken ∿16 hours at room temperature (∿22° C.). The octanol phase was drawn off and the water phase was placed in 250-ml polycarbonate centrifuge tubes and centrifuged at 10,000 rpm (13,700 x G) for 15 minutes. Following centrifugation, 600 ml of the water phase was transferred by pipet to a separatory funnel where it was, in turn, drawn off into a second separatory funnel to ensure the removal of octanol contamination transferred by the pipetting procedure.

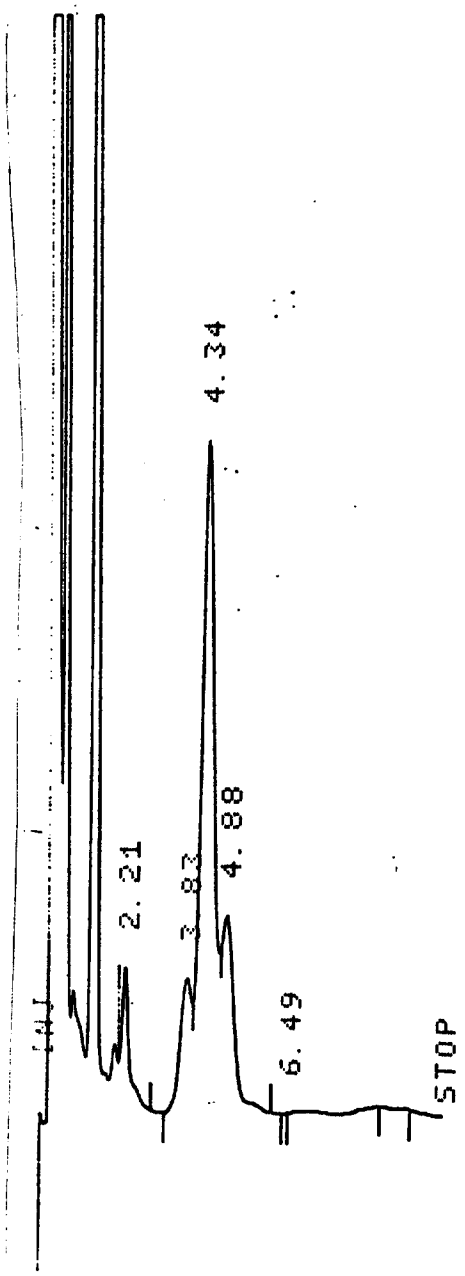

Figure 1. Gas Chromatogram of a 5 µl injection of a 1 ppm solution of FM 3925 (#081, 7/13/78). Peaks at 3.83, 4.34, and 4.88 minutes represent FM 3925. Gas chromatographic conditions are given in text.

The water phase was extracted three times with ethyl acetate, and the ethyl acetate extract was concentrated to 15 ml at room temperature under nitrogen. The FM 3925 concentration in the ethyl acetate was determined by electron capture gas chromatography. A typical gas chromatogram of the water phase is shown in Figure 2. The octanol phase from the distribution coefficient determination was not analyzed for FM 3925 content. Its FM 3925 concentration was assumed to be unchanged. This assumption was justified since measurement of the FM 3925 content from the octanol phase from previous attempts to determine the distribution coefficient had shown that the FM 3925 concentration was not detectably lowered by water extraction. A gas chromatogram showing the octanol phase after extraction is shown in Figure 3.

Results and Discussions

FM 3925 concentrations in the water phases shaken with the 1000 ppm and 2000 ppm FM 3925 n-octanol solutions were 0.0189 ppm and 0.033 ppm respectively. This data corresponds to distribution coefficients of 52,900 and 60,600. The average distribution coefficient for FM 3925 in n-octanol/water is 56,800.

Based on the method of Neely, Branson & Blair (3), this corresponds to a predicted bioconcentration factor between fish muscles and water of 500. Our laboratory findings on the structurally similar compound, FM 3422, gave values in this same range (4). Total body accumulation of FM 3422 into juvenile channel catfish indicated a bioconcentration factor of ∿500. Upon transfer to clear water, there was 50% clearance of the bioconcentrated FM 3422 within four days.

The lower distribution coefficient for FM 3925 compared to FM 3422 (56,800 vs. >100,000), and the greater water solubility of FM 3925 (0.82 mg/l vs. 0.05 mg/l) (5), suggest that FM 3925 will bioconcentrate to a lesser extent than FM 3422.

References:

(1) Burnett, R. Science 174:606, 1971.

(2) Gustafson, C. G. Env. Sci. & Tech. 4:814, 1970.

(3) Neely, W. B., D. R. Branson, and G. E. Blair, Env. Sci. & Tech. 8:1113, 1974.

(4) Welter, A. N. Evaluation of the Bioconcentration Potential of FM 3422, 3M Technical Report, August 16, 1978.

(5) Welter, A. N., E. A. Reiner, Solubility of FM 3925, 3M Technical Report, January 8, 1979.

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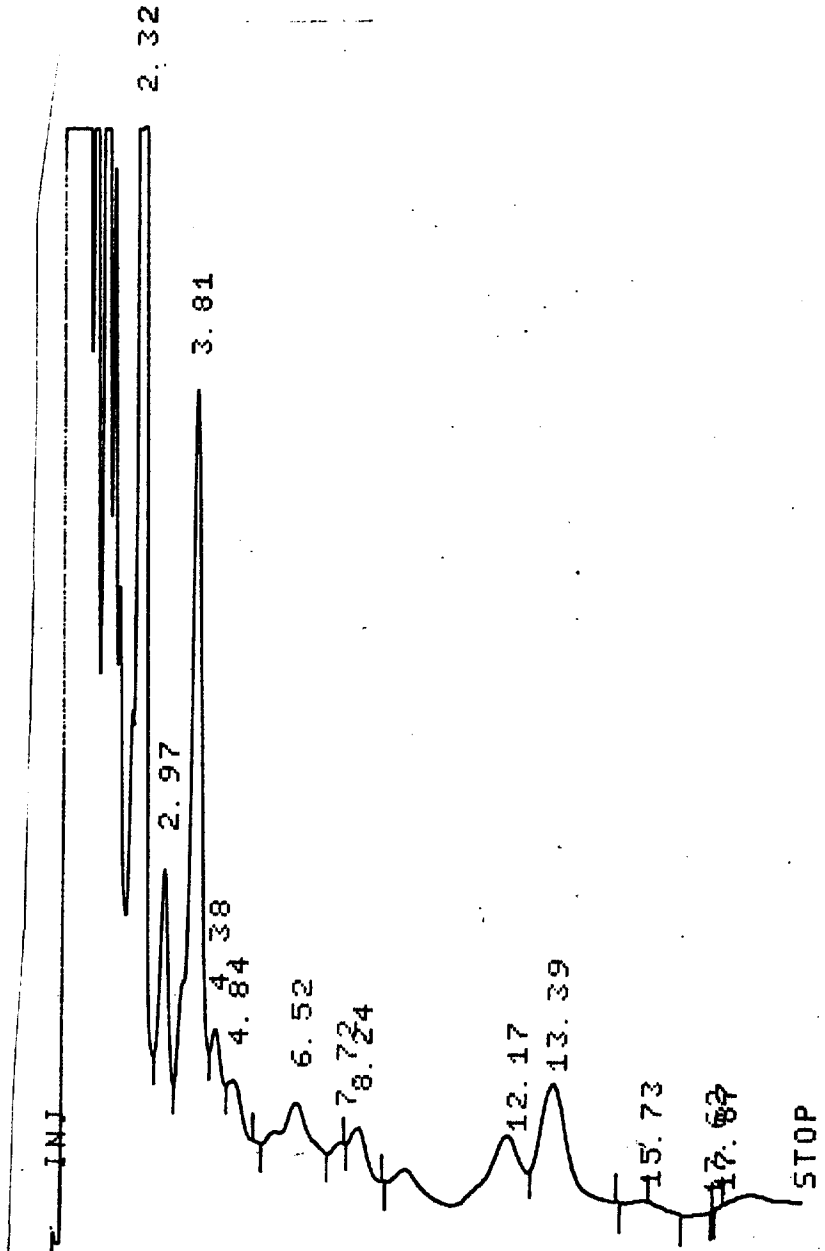

Figure 2. Gas Chromatogram of the water phase from an n-octanol/water distribution coefficient for FM 3925 (#082, 7/13/78). Peaks at 3.81, 4.38, and 4.84 minutes are taken to represent FM 3925. Gas chromatographic conditions are

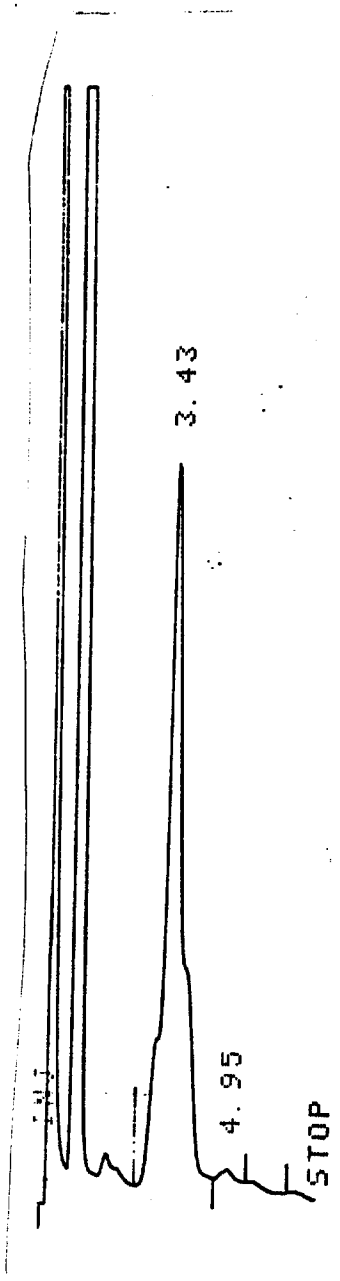

Figure 3. Gas Chromatogram of the octanol phase from an n-octanol/water distribution coefficient determination for FM 3925 (#163, 6/20/78). The peak at 3.43 minutes and shoulders before and after this peak represent FM 3925. Gas Chromatographic conditions are given in text.