

SOLUBILITY IN OCTANOL– SHAKE FLASK METHOD

TEST SUBSTANCE

Identity: Perfluorooctanesulfonate; may also be referred to as PFOS or FC-95. (1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-, potassium salt, CAS # 2795-39-3)

Remarks: The test substance is a white powder. Sample was re-crystallized from a production lot of FC-95, and assigned a test, control, and reference number TCR 00017-046. Purity determined to be 97.9% by LC/MS, ¹H-NMR, ¹⁹F-NMR and elemental analyses techniques.

METHOD

Method: Based on OECD 105, OPPTS 830.7840.

GLP (Y/N): Yes

Year completed: 2001

Octanol Source: Aldrich

Screen Test: Lot JU0873804, 99+%

Definitive Test: Lot 06238CI, 99.9+% HPLC Grade

Remarks: The definitive test consisted of placing ~0.010 g test substance with ~10 mL octanol in centrifuge tubes. The tubes were shaken at ~150 rpm at ~30°C for 24, 48 or 72-hours followed by 24-hours of equilibration at 22 - 23°C. Following equilibration, samples were centrifuged and the supernatant was analyzed by high performance liquid chromatography with mass spectrometric detection (LCMS).

RESULTS

24-hours: 56.9 mg/L

48-hours: 55.7 mg/L

72-hours: 55.4 mg/L

Mean solubility of PFOS in octanol = 56.0 mg/L

The 24, 48, and 72-hour solubility concentrations were averaged to obtain the overall mean solubility concentration

CONCLUSIONS

The overall mean solubility concentration of the test substance in pure octanol was 56.0 mg/L.

Typically, the Column Elution Method is recommended for use with substances with solubility screening results of < 10 mg/L. However, the shake flask method was utilized in this study because of the difficulty in obtaining tubing compatible with octanol and the possible explosion hazard posed by possible leaks of a flammable solvent in an incubator.

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

DATA QUALITY

Reliability: Klimisch ranking 1.

REFERENCES

Studies conducted at the 3M Company, St Paul, MN, 2001, Environmental Laboratory Project Number EOO-1716.

OTHER

Last changed: 6/22/01