COMPARISON OF PROPOSED HHBAFs FOR THE GLI

by

Charles E. Stephan

Environmental Research Laboratory
Office of Research and Development
U.S. Environmental Protection Agency
Duluth, MN

[redacted]

> No measured BAF was found.

2,4,6-TRICHLOROPHENOL [CAS#: 88-06-2]

> Predicted BAF based on Log P:
The following values were found for Log P:

3.69	MedChem Star
3.57	MedChem Calc
2.97	Isnard and Lambert 1989

A value of 3.5 was selected as a "typical Log P", from which the following were obtained:
Predicted BCF (at 7.6% lipids) = 231.7
Normalized BCF (at 1.0% lipids) = 30.5
Food Chain Multiplier = 1.0
For 5.0% lipids at trophic level 4 the predicted HHBAF that is calculated from the "typical Log P" is (30.5)(5.0)(1.0) = 152.

> Predicted BAF based on Log P and measured BCF:

BCF	% L	Norm BCF (1.0% L)	Reference
88	12.4	7.10	Smith et al. 1990,1991

Geometric mean normalized BCF = 7.10

For 5.0% lipids at trophic level 4 the predicted HHBAF that is calculated from the geometric mean normalized BCF is (7.10)(5.0)(1.0) = 36.

> No measured BAF was found.

VINYL CHLORIDE [CAS#: 75-01-4]

> Predicted BAF based on Log P:
The following value was found for Log P:

1.36	MedChem Calc

A value of 1.36 was selected as a "typical Log P", from which the following were obtained:
Predicted BCF (at 7.6% lipids) = 4.72
Normalized BCF (at 1.0% lipids) = 0.621
Food Chain Multiplier = 1.0
For 5.0% lipids at trophic level 4 the predicted HHBAF that is calculated from the "typical Log P" is (0.621)(5.0)(1.0) = 3.1.