

SMILES : c1ccc(cc1)c2ccc(cc2)CC

CHEM :

MOL FOR: C14 H14

MOL WT : 182.27

----- BCFBAF v3.01 -----

Summary Results:

Log BCF (regression-based estimate): 2.83 (BCF = 678 L/kg wet-wt)  
Biotransformation Half-Life (days) : 6.58 (normalized to 10 g fish)  
Log BAF (Arnot-Gobas upper trophic): 2.65 (BAF = 451 L/kg wet-wt)

Experimental BCF-kM Database Structure Match:

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Name : 4-Ethylbiphenyl  
CAS Num : 005707-44-8  
Log BCF : 2.8241 (BCF = 667 L/kg wet-wt)  
BCF Data : BCF NonIonic Training Set  
Log Bio HL: 0.064 (Bio Half-life = 1.16 days)  
Bio Data : kM Training Set

Log Kow (experimental): not available from database

Log Kow used by BCF estimates: 4.80

Equation Used to Make BCF estimate:

Log BCF = 0.6598 log Kow - 0.333 + Correction

Correction(s): Value

No Applicable Correction Factors

Estimated Log BCF = 2.831 (BCF = 677.6 L/kg wet-wt)

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Whole Body Primary Biotransformation Rate Estimate for Fish:  
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TYPE	NUM	LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Alkyl substituent on aromatic ring	0.1781	0.1781
Frag	1	Unsubstituted phenyl group (C6H5-)	-0.6032	-0.6032
Frag	1	Aromatic-CH2	-0.3365	-0.3365
Frag	9	Aromatic-H	0.2664	2.3974
Frag	1	Methyl [-CH3]	0.2451	0.2451
Frag	1	Biphenyl	-0.5319	-0.5319
L Kow	*	Log Kow = 4.80 (KowWin estimate)	0.3073	1.4738
MolWt	*	Molecular Weight Parameter		-0.4674
Const	*	Equation Constant		-1.5058
RESULT		LOG Bio Half-Life (days)		0.8183
RESULT		Bio Half-Life (days)		6.581
NOTE		Bio Half-Life Normalized to 10 g fish at 15 deg C		

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Biotransformation Rate Constant:

kM (Rate Constant): 0.1053 /day (10 gram fish)  
kM (Rate Constant): 0.05923 /day (100 gram fish)  
kM (Rate Constant): 0.03331 /day (1 kg fish)  
kM (Rate Constant): 0.01873 /day (10 kg fish)

Note: For Arnot-Gobas BCF & BAF Methods, Experimental Km Half-Life Used:

Exp Km Half-Life = 0.064 days (Rate Constant = 0.5982/ day)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):

Estimated Log BCF (upper trophic) = 2.653 (BCF = 449.4 L/kg wet-wt)

Estimated Log BAF (upper trophic) = 2.655 (BAF = 451.4 L/kg wet-wt)

Estimated Log BCF (mid trophic) = 2.759 (BCF = 573.9 L/kg wet-wt)  
 Estimated Log BAF (mid trophic) = 2.779 (BAF = 601.6 L/kg wet-wt)  
 Estimated Log BCF (lower trophic) = 2.786 (BCF = 611.3 L/kg wet-wt)  
 Estimated Log BAF (lower trophic) = 2.863 (BAF = 729.7 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):

Estimated Log BCF (upper trophic) = 3.738 (BCF = 5468 L/kg wet-wt)  
 Estimated Log BAF (upper trophic) = 4.689 (BAF = 4.883e+004 L/kg wet-wt)

SMILES : c1ccc(cc1)C  
 CHEM :  
 MOL FOR: C7 H8  
 MOL WT : 92.14

----- BCFBAF v3.01 -----

Summary Results:

Log BCF (regression-based estimate): 1.47 (BCF = 29.4 L/kg wet-wt)  
 Biotransformation Half-Life (days) : 0.287 (normalized to 10 g fish)  
 Log BAF (Arnot-Gobas upper trophic): 1.58 (BAF = 37.8 L/kg wet-wt)

Experimental BCF-kM Database Structure Match:

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 Name : Benzene, methyl-  
 CAS Num : 000108-88-3  
 Log BCF : 0.92 (BCF = 8.32 L/kg wet-wt)  
 BCF Data : BCF Validation Set  
 Log Bio HL: ---  
 Bio Data : ---

Log Kow (experimental): 2.73  
 Log Kow used by BCF estimates: 2.73

Equation Used to Make BCF estimate:

$$\text{Log BCF} = 0.6598 \log \text{Kow} - 0.333 + \text{Correction}$$

Correction(s): Value  
 No Applicable Correction Factors

Estimated Log BCF = 1.468 (BCF = 29.39 L/kg wet-wt)

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 Whole Body Primary Biotransformation Rate Estimate for Fish:  
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TYPE	NUM	LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Alkyl substituent on aromatic ring	0.1781	0.1781
Frag	1	Unsubstituted phenyl group (C6H5-)	-0.6032	-0.6032
Frag	1	Aromatic-CH3	-0.0872	-0.0872
Frag	5	Aromatic-H	0.2664	1.3319
Frag	1	Benzene	-0.4277	-0.4277
L Kow	*	Log Kow = 2.73 (experimental )	0.3073	0.8390
MolWt	*	Molecular Weight Parameter		-0.2363
Const	*	Equation Constant		-1.5058
RESULT		LOG Bio Half-Life (days)		-0.5424
RESULT		Bio Half-Life (days)		0.2868
NOTE		Bio Half-Life Normalized to 10 g fish at 15 deg C		

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Biotransformation Rate Constant:

kM (Rate Constant): 2.417 /day (10 gram fish)  
 kM (Rate Constant): 1.359 /day (100 gram fish)  
 kM (Rate Constant): 0.7643 /day (1 kg fish)  
 kM (Rate Constant): 0.4298 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):

Estimated Log BCF (upper trophic) = 1.577 (BCF = 37.79 L/kg wet-wt)  
 Estimated Log BAF (upper trophic) = 1.577 (BAF = 37.79 L/kg wet-wt)  
 Estimated Log BCF (mid trophic) = 1.479 (BCF = 30.13 L/kg wet-wt)  
 Estimated Log BAF (mid trophic) = 1.479 (BAF = 30.14 L/kg wet-wt)  
 Estimated Log BCF (lower trophic) = 1.441 (BCF = 27.58 L/kg wet-wt)  
 Estimated Log BAF (lower trophic) = 1.441 (BAF = 27.6 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):

Estimated Log BCF (upper trophic) = 1.765 (BCF = 58.23 L/kg wet-wt)  
 Estimated Log BAF (upper trophic) = 1.798 (BAF = 62.87 L/kg wet-wt)

SMILES : CCC(C)CC(C)(CC)c1cc(Br)c(O)cc1

CHEM :

MOL FOR: C15 H23 Br1 O1

MOL WT : 299.25

----- BCFBAF v3.01 -----

Summary Results:

Log BCF (regression-based estimate): 4.08 (BCF = 1.21e+004 L/kg wet-wt)  
 Biotransformation Half-Life (days) : 4.09 (normalized to 10 g fish)  
 Log BAF (Arnot-Gobas upper trophic): 3.56 (BAF = 3.61e+003 L/kg wet-wt)

Log Kow (experimental): not available from database

Log Kow used by BCF estimates: 6.69

Equation Used to Make BCF estimate:

$$\text{Log BCF} = 0.6598 \text{ log Kow} - 0.333 + \text{Correction}$$

Correction(s): Value  
 No Applicable Correction Factors

Estimated Log BCF = 4.084 (BCF = 1.213e+004 L/kg wet-wt)

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 Whole Body Primary Biotransformation Rate Estimate for Fish:  
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TYPE	NUM	LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	-0.4727	-0.4727
Frag	1	Aromatic bromide [-Br]	0.3964	0.3964
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.2984	-0.2984
Frag	3	Aromatic-H	0.2664	0.7991
Frag	4	Methyl [-CH3]	0.2451	0.9804
Frag	3	-CH2- [linear]	0.0242	0.0726
Frag	1	-CH- [linear]	-0.1912	-0.1912
Frag	1	Benzene	-0.4277	-0.4277
L Kow	*	Log Kow = 6.69 (KowWin estimate)	0.3073	2.0574
MolWt	*	Molecular Weight Parameter		-0.7674
Const	*	Equation Constant		-1.5058
RESULT		LOG Bio Half-Life (days)		0.6113
RESULT		Bio Half-Life (days)		4.086

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Biotransformation Rate Constant:

kM (Rate Constant): 0.1696 /day (10 gram fish)  
kM (Rate Constant): 0.09539 /day (100 gram fish)  
kM (Rate Constant): 0.05364 /day (1 kg fish)  
kM (Rate Constant): 0.03016 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):

Estimated Log BCF (upper trophic) = 2.907 (BCF = 806.4 L/kg wet-wt)  
Estimated Log BAF (upper trophic) = 3.558 (BAF = 3613 L/kg wet-wt)  
Estimated Log BCF (mid trophic) = 3.046 (BCF = 1113 L/kg wet-wt)  
Estimated Log BAF (mid trophic) = 4.139 (BAF = 1.377e+004 L/kg wet-wt)  
Estimated Log BCF (lower trophic) = 3.089 (BCF = 1227 L/kg wet-wt)  
Estimated Log BAF (lower trophic) = 4.497 (BAF = 3.139e+004 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):

Estimated Log BCF (upper trophic) = 4.210 (BCF = 1.621e+004 L/kg wet-wt)  
Estimated Log BAF (upper trophic) = 6.958 (BAF = 9.082e+006 L/kg wet-wt)