

SMILES : Oc1ccc(cc1)C(C)(C)c2ccc(cc2)O  
 CHEM :  
 MOL FOR: C15 H16 O2  
 MOL WT : 228.29

----- BIOWIN v4.10 Results -----

Biowin1 (Linear Model Prediction) : Biodegrades Fast  
 Biowin2 (Non-Linear Model Prediction): Does Not Biodegrade Fast  
 Biowin3 (Ultimate Biodegradation Timeframe): Weeks-Months  
 Biowin4 (Primary Biodegradation Timeframe): Days-Weeks  
 Biowin5 (MITI Linear Model Prediction) : Not Readily Degradable  
 Biowin6 (MITI Non-Linear Model Prediction): Not Readily Degradable  
 Biowin7 (Anaerobic Model Prediction): Does Not Biodegrade Fast  
 Ready Biodegradability Prediction: NO

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag	2	Aromatic alcohol [-OH]	0.1158	0.2316	
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.1839	-0.1839	
MolWt	*	Molecular Weight Parameter		-0.1087	
Const	*	Equation Constant		0.7475	
RESULT				Biowin1 (Linear Biodeg Probability)	0.6866

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag	2	Aromatic alcohol [-OH]	0.9086	1.8172	
Frag	1	Carbon with 4 single bonds & no hydrogens	-1.7232	-1.7232	
MolWt	*	Molecular Weight Parameter		-3.2418	
RESULT				Biowin2 (Non-Linear Biodeg Probability)	0.4653

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag	2	Aromatic alcohol [-OH]	0.0564	0.1128	
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.2121	-0.2121	
MolWt	*	Molecular Weight Parameter		-0.5045	
Const	*	Equation Constant		3.1992	
RESULT				Biowin3 (Survey Model - Ultimate Biodeg)	2.5953

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.0397	0.0794
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.1534	-0.1534

MolWt	*	Molecular Weight Parameter		-0.3294
Const	*	Equation Constant		3.8477
=====				
RESULT		Biowin4 (Survey Model - Primary Biodeg)		3.4443
=====				

Result Classification: 5.00 -> hours      4.00 -> days      3.00 -> weeks  
 (Primary & Ultimate) 2.00 -> months      1.00 -> longer

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.0642	0.1285
Frag	1	Carbon with 4 single bonds & no hydrogens	0.0676	0.0676
Frag	8	Aromatic-H	0.0082	0.0657
Frag	2	Methyl [-CH3]	0.0004	0.0008
MolWt	*	Molecular Weight Parameter		-0.6792
Const	*	Equation Constant		0.7121
=====				
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.2956
=====				

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.4884	0.9768
Frag	1	Carbon with 4 single bonds & no hydrogens	0.3990	0.3990
Frag	8	Aromatic-H	0.1201	0.9611
Frag	2	Methyl [-CH3]	0.0194	0.0389
MolWt	*	Molecular Weight Parameter		-6.5905
=====				
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.1559
=====				

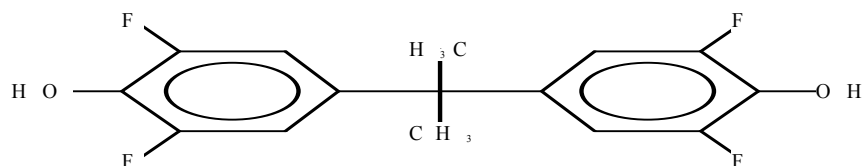
A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable  
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.0807	0.1614
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.3342	-0.3342
Frag	8	Aromatic-H	-0.0954	-0.7634
Frag	2	Methyl [-CH3]	-0.0796	-0.1591
Const	*	Equation Constant		0.8361
=====				
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		-0.2593
=====				

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is  $\geq 0.5$ , then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.



SMILES : Oc1c(F)cc(cc1F)C(C)(C)c2cc(F)c(c(F)c2)O  
 CHEM :  
 MOL FOR: C15 H12 F4 O2  
 MOL WT : 300.25

----- BIOWIN v4.10 Results -----

Biowin1 (Linear Model Prediction) : Does Not Biodegrade Fast  
 Biowin2 (Non-Linear Model Prediction): Does Not Biodegrade Fast  
 Biowin3 (Ultimate Biodegradation Timeframe): Recalcitrant  
 Biowin4 (Primary Biodegradation Timeframe): Days-Weeks  
 Biowin5 (MITI Linear Model Prediction) : Not Readily Degradable  
 Biowin6 (MITI Non-Linear Model Prediction): Not Readily Degradable  
 Biowin7 (Anaerobic Model Prediction): Does Not Biodegrade Fast  
 Ready Biodegradability Prediction: NO

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.1158	0.2316
Frag	4	Aromatic fluoride [-F]	-0.8100	-3.2400
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.1839	-0.1839
MolWt	*	Molecular Weight Parameter		-0.1429
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		-2.5877

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.9086	1.8172
Frag	4	Aromatic fluoride [-F]	-10.5318	-42.1272
Frag	1	Carbon with 4 single bonds & no hydrogens	-1.7232	-1.7232
MolWt	*	Molecular Weight Parameter		-4.2636
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.0000

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.0564	0.1128
Frag	4	Aromatic fluoride [-F]	-0.4069	-1.6278
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.2121	-0.2121
MolWt	*	Molecular Weight Parameter		-0.6635
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		0.8085

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
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Frag	2	Aromatic alcohol [-OH]	0.0397	0.0794
Frag	4	Aromatic fluoride [-F]	0.0135	0.0538
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.1534	-0.1534
MolWt	*	Molecular Weight Parameter		-0.4332
Const	*	Equation Constant		3.8477
=====				
RESULT		Biowin4 (Survey Model - Primary Biodeg)		3.3943
=====				

Result Classification: 5.00 -> hours      4.00 -> days      3.00 -> weeks  
 (Primary & Ultimate)    2.00 -> months      1.00 -> longer

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.0642	0.1285
Frag	1	Carbon with 4 single bonds & no hydrogens	0.0676	0.0676
Frag	4	Fluorine [-F]	0.0174	0.0695
Frag	4	Aromatic-H	0.0082	0.0329
Frag	2	Methyl [-CH3]	0.0004	0.0008
MolWt	*	Molecular Weight Parameter		-0.8933
Const	*	Equation Constant		0.7121
=====				
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.1182
=====				

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.4884	0.9768
Frag	1	Carbon with 4 single bonds & no hydrogens	0.3990	0.3990
Frag	4	Fluorine [-F]	-3.9878	-15.9514
Frag	4	Aromatic-H	0.1201	0.4806
Frag	2	Methyl [-CH3]	0.0194	0.0389
MolWt	*	Molecular Weight Parameter		-8.6680
=====				
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.0000
=====				

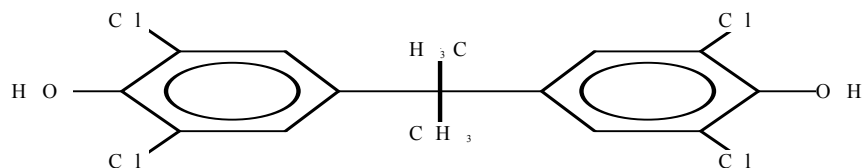
A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable  
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.0807	0.1614
Frag	4	Aromatic fluoride [-F]	0.0000	0.0000
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.3342	-0.3342
Frag	4	Fluorine [-F]	0.0000	0.0000
Frag	4	Aromatic-H	-0.0954	-0.3817
Frag	2	Methyl [-CH3]	-0.0796	-0.1591
Const	*	Equation Constant		0.8361
=====				
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		0.1224
=====				

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is  $\geq 0.5$ , then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for



SMILES : Oc1c(Cl)cc(cc1CL)C(C)(C)c2cc(Cl)c(c(Cl)c2)O  
 CHEM :  
 MOL FOR: C15 H12 CL4 O2  
 MOL WT : 366.07

----- BIOWIN v4.10 Results -----

Biowin1 (Linear Model Prediction) : Does Not Biodegrade Fast  
 Biowin2 (Non-Linear Model Prediction): Does Not Biodegrade Fast  
 Biowin3 (Ultimate Biodegradation Timeframe): Recalcitrant  
 Biowin4 (Primary Biodegradation Timeframe): Weeks-Months  
 Biowin5 (MITI Linear Model Prediction) : Not Readily Degradable  
 Biowin6 (MITI Non-Linear Model Prediction): Not Readily Degradable  
 Biowin7 (Anaerobic Model Prediction): Does Not Biodegrade Fast  
 Ready Biodegradability Prediction: NO

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.1158	0.2316
Frag	4	Aromatic chloride [-CL]	-0.1824	-0.7297
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.1839	-0.1839
MolWt	*	Molecular Weight Parameter		-0.1743
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		-0.1087

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.9086	1.8172
Frag	4	Aromatic chloride [-CL]	-2.0155	-8.0620
Frag	1	Carbon with 4 single bonds & no hydrogens	-1.7232	-1.7232
MolWt	*	Molecular Weight Parameter		-5.1982
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.0000

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.0564	0.1128
Frag	4	Aromatic chloride [-CL]	-0.2066	-0.8264
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.2121	-0.2121
MolWt	*	Molecular Weight Parameter		-0.8090
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		1.4644

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
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Frag	2	Aromatic alcohol [-OH]	0.0397	0.0794
Frag	4	Aromatic chloride [-CL]	-0.1653	-0.6614
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.1534	-0.1534
MolWt	*	Molecular Weight Parameter		-0.5282
Const	*	Equation Constant		3.8477
=====				
RESULT		Biowin4 (Survey Model - Primary Biodeg)		2.5842
=====				

Result Classification: 5.00 -> hours      4.00 -> days      3.00 -> weeks  
 (Primary & Ultimate)    2.00 -> months      1.00 -> longer

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.0642	0.1285
Frag	4	Aromatic chloride [-CL]	0.0062	0.0247
Frag	1	Carbon with 4 single bonds & no hydrogens	0.0676	0.0676
Frag	4	Aromatic-H	0.0082	0.0329
Frag	2	Methyl [-CH3]	0.0004	0.0008
MolWt	*	Molecular Weight Parameter		-1.0891
Const	*	Equation Constant		0.7121
=====				
RESULT		Biowin5 (MITI Linear Biodeg Probability)		-0.1225
=====				

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.4884	0.9768
Frag	4	Aromatic chloride [-CL]	-0.2191	-0.8766
Frag	1	Carbon with 4 single bonds & no hydrogens	0.3990	0.3990
Frag	4	Aromatic-H	0.1201	0.4806
Frag	2	Methyl [-CH3]	0.0194	0.0389
MolWt	*	Molecular Weight Parameter		-10.5681
=====				
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.0009
=====				

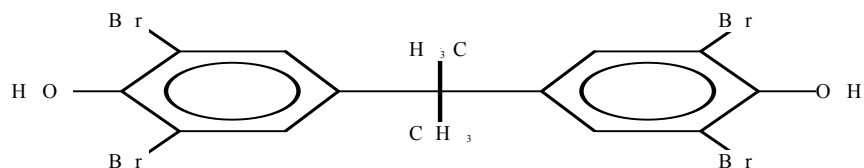
A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable  
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.0807	0.1614
Frag	4	Aromatic chloride [-CL]	-0.4023	-1.6091
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.3342	-0.3342
Frag	4	Aromatic-H	-0.0954	-0.3817
Frag	2	Methyl [-CH3]	-0.0796	-0.1591
Const	*	Equation Constant		0.8361
=====				
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		-1.4867
=====				

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is  $\geq 0.5$ , then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals



SMILES : Oc1c(Br)cc(cc1Br)C(C)(C)c2cc(Br)c(c(Br)c2)O  
 CHEM :  
 MOL FOR: C15 H12 Br4 O2  
 MOL WT : 543.88

----- BIOWIN v4.10 Results -----

Biowin1 (Linear Model Prediction) : Does Not Biodegrade Fast  
 Biowin2 (Non-Linear Model Prediction): Does Not Biodegrade Fast  
 Biowin3 (Ultimate Biodegradation Timeframe): Recalcitrant  
 Biowin4 (Primary Biodegradation Timeframe): Weeks-Months  
 Biowin5 (MITI Linear Model Prediction) : Not Readily Degradable  
 Biowin6 (MITI Non-Linear Model Prediction): Not Readily Degradable  
 Biowin7 (Anaerobic Model Prediction): Does Not Biodegrade Fast  
 Ready Biodegradability Prediction: NO

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag	2	Aromatic alcohol [-OH]	0.1158	0.2316	
Frag	4	Aromatic bromide [-Br]	-0.1103	-0.4414	
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.1839	-0.1839	
MolWt	*	Molecular Weight Parameter		-0.2589	
Const	*	Equation Constant		0.7475	
RESULT				Biowin1 (Linear Biodeg Probability)	0.0949

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag	2	Aromatic alcohol [-OH]	0.9086	1.8172	
Frag	4	Aromatic bromide [-Br]	-1.6779	-6.7116	
Frag	1	Carbon with 4 single bonds & no hydrogens	-1.7232	-1.7232	
MolWt	*	Molecular Weight Parameter		-7.7231	
RESULT				Biowin2 (Non-Linear Biodeg Probability)	0.0000

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag	2	Aromatic alcohol [-OH]	0.0564	0.1128	
Frag	4	Aromatic bromide [-Br]	-0.1360	-0.5440	
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.2121	-0.2121	
MolWt	*	Molecular Weight Parameter		-1.2019	
Const	*	Equation Constant		3.1992	
RESULT				Biowin3 (Survey Model - Ultimate Biodeg)	1.3539

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
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Frag	2	Aromatic alcohol [-OH]	0.0397	0.0794
Frag	4	Aromatic bromide [-Br]	-0.1535	-0.6140
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.1534	-0.1534
MolWt	*	Molecular Weight Parameter		-0.7847
Const	*	Equation Constant		3.8477
=====				
RESULT		Biowin4 (Survey Model - Primary Biodeg)		2.3750
=====				

Result Classification: 5.00 -> hours      4.00 -> days      3.00 -> weeks  
 (Primary & Ultimate)    2.00 -> months      1.00 -> longer

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.0642	0.1285
Frag	4	Aromatic bromide [-Br]	0.1668	0.6671
Frag	1	Carbon with 4 single bonds & no hydrogens	0.0676	0.0676
Frag	4	Aromatic-H	0.0082	0.0329
Frag	2	Methyl [-CH3]	0.0004	0.0008
MolWt	*	Molecular Weight Parameter		-1.6180
Const	*	Equation Constant		0.7121
=====				
RESULT		Biowin5 (MITI Linear Biodeg Probability)		-0.0090
=====				

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.4884	0.9768
Frag	4	Aromatic bromide [-Br]	1.5021	6.0085
Frag	1	Carbon with 4 single bonds & no hydrogens	0.3990	0.3990
Frag	4	Aromatic-H	0.1201	0.4806
Frag	2	Methyl [-CH3]	0.0194	0.0389
MolWt	*	Molecular Weight Parameter		-15.7011
=====				
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.0051
=====				

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable  
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

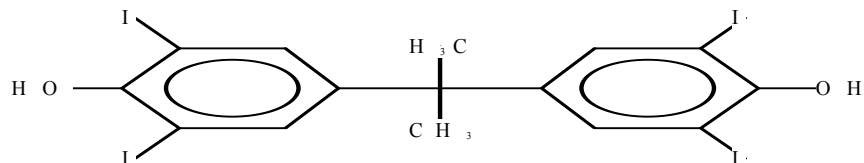
TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.0807	0.1614
Frag	4	Aromatic bromide [-Br]	0.0000	0.0000
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.3342	-0.3342
Frag	4	Aromatic-H	-0.0954	-0.3817
Frag	2	Methyl [-CH3]	-0.0796	-0.1591
Const	*	Equation Constant		0.8361
=====				
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		0.1224
=====				

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is  $\geq 0.5$ , then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals





SMILES : Oc1c(I)cc(cc1I)C(C)(C)c2cc(I)c(c(I)c2)O  
 CHEM :  
 MOL FOR: C15 H12 I4 O2  
 MOL WT : 731.88

----- BIOWIN v4.10 Results -----

Biowin1 (Linear Model Prediction) : Does Not Biodegrade Fast  
 Biowin2 (Non-Linear Model Prediction): Does Not Biodegrade Fast  
 Biowin3 (Ultimate Biodegradation Timeframe): Recalcitrant  
 Biowin4 (Primary Biodegradation Timeframe): Months  
 Biowin5 (MITI Linear Model Prediction) : Not Readily Degradable  
 Biowin6 (MITI Non-Linear Model Prediction): Not Readily Degradable  
 Biowin7 (Anaerobic Model Prediction): Does Not Biodegrade Fast  
 Ready Biodegradability Prediction: NO

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.1158	0.2316
Frag	4	Aromatic iodide [-I]	-0.7586	-3.0345
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.1839	-0.1839
MolWt	*	Molecular Weight Parameter		-0.3484
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		-2.5877

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.9086	1.8172
Frag	4	Aromatic iodide [-I]	-10.0033	-40.0132
Frag	1	Carbon with 4 single bonds & no hydrogens	-1.7232	-1.7232
MolWt	*	Molecular Weight Parameter		-10.3927
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.0000

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.0564	0.1128
Frag	4	Aromatic iodide [-I]	-0.0449	-0.1798
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.2121	-0.2121
MolWt	*	Molecular Weight Parameter		-1.6174
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		1.3027

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
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Frag	2	Aromatic alcohol [-OH]	0.0397	0.0794
Frag	4	Aromatic iodide [-I]	-0.1271	-0.5083
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.1534	-0.1534
MolWt	*	Molecular Weight Parameter		-1.0559
Const	*	Equation Constant		3.8477
=====				
RESULT		Biowin4 (Survey Model - Primary Biodeg)		2.2095
=====				

Result Classification: 5.00 -> hours      4.00 -> days      3.00 -> weeks  
 (Primary & Ultimate)    2.00 -> months      1.00 -> longer

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.0642	0.1285
Frag	4	Aromatic iodide [-I]	-0.3840	-1.5361
Frag	1	Carbon with 4 single bonds & no hydrogens	0.0676	0.0676
Frag	4	Aromatic-H	0.0082	0.0329
Frag	2	Methyl [-CH3]	0.0004	0.0008
MolWt	*	Molecular Weight Parameter		-2.1773
Const	*	Equation Constant		0.7121
=====				
RESULT		Biowin5 (MITI Linear Biodeg Probability)		-2.7715
=====				

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.4884	0.9768
Frag	4	Aromatic iodide [-I]	-12.5224	-50.0895
Frag	1	Carbon with 4 single bonds & no hydrogens	0.3990	0.3990
Frag	4	Aromatic-H	0.1201	0.4806
Frag	2	Methyl [-CH3]	0.0194	0.0389
MolWt	*	Molecular Weight Parameter		-21.1284
=====				
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.0000
=====				

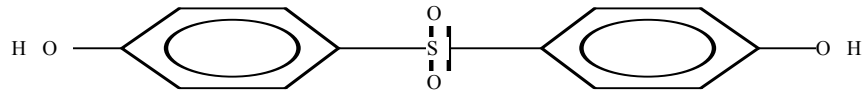
A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable  
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.0807	0.1614
Frag	4	Aromatic iodide [-I]	0.0000	0.0000
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.3342	-0.3342
Frag	4	Aromatic-H	-0.0954	-0.3817
Frag	2	Methyl [-CH3]	-0.0796	-0.1591
Const	*	Equation Constant		0.8361
=====				
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		0.1224
=====				

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is  $\geq 0.5$ , then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals



SMILES : Oc1ccc(cc1)S(=O)(=O)c2ccc(O)cc2  
 CHEM :  
 MOL FOR: C12 H10 O4 S1  
 MOL WT : 250.27

----- BIOWIN v4.10 Results -----

Biowin1 (Linear Model Prediction) : Biodegrades Fast  
 Biowin2 (Non-Linear Model Prediction): Biodegrades Fast  
 Biowin3 (Ultimate Biodegradation Timeframe): Weeks  
 Biowin4 (Primary Biodegradation Timeframe): Days-Weeks  
 Biowin5 (MITI Linear Model Prediction) : Not Readily Degradable  
 Biowin6 (MITI Non-Linear Model Prediction): Not Readily Degradable  
 Biowin7 (Anaerobic Model Prediction): Does Not Biodegrade Fast  
 Ready Biodegradability Prediction: NO

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag	2	Aromatic alcohol [-OH]	0.1158	0.2316	
MolWt	*	Molecular Weight Parameter		-0.1191	
Const	*	Equation Constant		0.7475	
RESULT				Biowin1 (Linear Biodeg Probability)	0.8600

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag	2	Aromatic alcohol [-OH]	0.9086	1.8172	
MolWt	*	Molecular Weight Parameter		-3.5538	
RESULT				Biowin2 (Non-Linear Biodeg Probability)	0.7811

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag	2	Aromatic alcohol [-OH]	0.0564	0.1128	
MolWt	*	Molecular Weight Parameter		-0.5531	
Const	*	Equation Constant		3.1992	
RESULT				Biowin3 (Survey Model - Ultimate Biodeg)	2.7589

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag	2	Aromatic alcohol [-OH]	0.0397	0.0794	
MolWt	*	Molecular Weight Parameter		-0.3611	
Const	*	Equation Constant		3.8477	
RESULT				Biowin4 (Survey Model - Primary Biodeg)	3.5660

Result Classification: 5.00 -> hours      4.00 -> days      3.00 -> weeks  
 (Primary & Ultimate)    2.00 -> months      1.00 -> longer

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.0642	0.1285
Frag	8	Aromatic-H	0.0082	0.0657
MolWt	*	Molecular Weight Parameter		-0.7446
Const	*	Equation Constant		0.7121
RESULT			Biowin5 (MITI Linear Biodeg Probability)	0.1618

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.4884	0.9768
Frag	8	Aromatic-H	0.1201	0.9611
MolWt	*	Molecular Weight Parameter		-7.2250
RESULT			Biowin6 (MITI Non-Linear Biodeg Probability)	0.0594

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable  
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.0807	0.1614
Frag	8	Aromatic-H	-0.0954	-0.7634
Const	*	Equation Constant		0.8361
RESULT			Biowin7 (Anaerobic Linear Biodeg Prob)	0.2341

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is  $\geq 0.5$ , then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.