

SMILES : c12cccc1cccc2
 CHEM :
 MOL FOR: C10 H8
 MOL WT : 128.18

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

Biowin1 (Linear Model Prediction) : Biodegrades Fast
 Biowin2 (Non-Linear Model Prediction): Biodegrades 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	1	Unsubstituted aromatic (3 or less rings)	0.3192	0.3192
MolWt	*	Molecular Weight Parameter		-0.0610
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		1.0057

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Unsubstituted aromatic (3 or less rings)	7.1908	7.1908
MolWt	*	Molecular Weight Parameter		-1.8201
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.9998

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	1	Unsubstituted aromatic (3 or less rings)	-0.5859	-0.5859
MolWt	*	Molecular Weight Parameter		-0.2832
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		2.3300

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Unsubstituted aromatic (3 or less rings)	-0.3428	-0.3428
MolWt	*	Molecular Weight Parameter		-0.1849
Const	*	Equation Constant		3.8477
RESULT		Biowin4 (Survey Model - Primary Biodeg)		3.3200

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	8	Aromatic-H	0.0082	0.0657
MolWt	*	Molecular Weight Parameter		-0.3813
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.3966

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	8	Aromatic-H	0.1201	0.9611
MolWt	*	Molecular Weight Parameter		-3.7003
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.4468

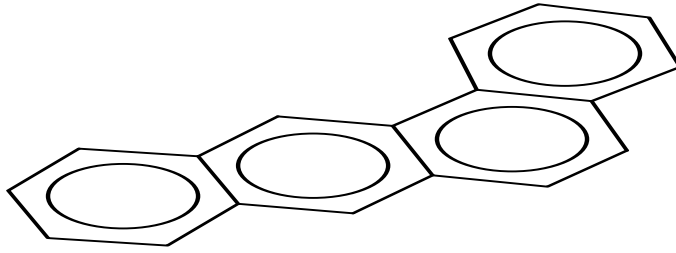
A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Unsubstituted aromatic (3 or less rings)	-0.2635	-0.2635
Frag	8	Aromatic-H	-0.0954	-0.7634
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		-0.1909

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 ≥ 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 : c12ccc3c(cc(cccc4)c4c3)c1cccc2
 CHEM :
 MOL FOR: C18 H12
 MOL WT : 228.30

----- 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): Months
 Biowin4 (Primary Biodegradation Timeframe): 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	1	Polyaromatic hydrocarbon (4 or more rings)	-0.6573	-0.6573
MolWt	*	Molecular Weight Parameter		-0.1087
Const	*	Equation Constant		0.7475
RESULT				-0.0184

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Polyaromatic hydrocarbon (4 or more rings)	-10.1644	-10.1644
MolWt	*	Molecular Weight Parameter		-3.2418
RESULT				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	1	Polyaromatic hydrocarbon (4 or more rings)	-0.7993	-0.7993
MolWt	*	Molecular Weight Parameter		-0.5045
Const	*	Equation Constant		3.1992
RESULT				1.8953

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Polyaromatic hydrocarbon (4 or more rings)	-0.7022	-0.7022
MolWt	*	Molecular Weight Parameter		-0.3294
Const	*	Equation Constant		3.8477
RESULT				2.8161

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	12	Aromatic-H	0.0082	0.0986
MolWt	*	Molecular Weight Parameter		-0.6792
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.1316

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	12	Aromatic-H	0.1201	1.4417
MolWt	*	Molecular Weight Parameter		-6.5906
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.0677

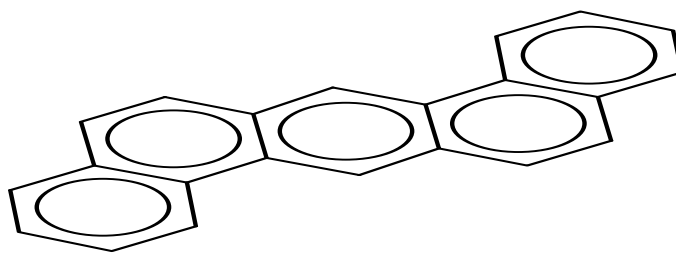
A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Polyaromatic hydrocarbon (4 or more rings)	0.0000	0.0000
Frag	12	Aromatic-H	-0.0954	-1.1452
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		-0.3091

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 ≥ 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 : c12ccc3c(cc(ccc4c5cccc4)c5c3)c1cccc2
 CHEM :
 MOL FOR: C22 H14
 MOL WT : 278.36

----- 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): Months
 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	1	Polyaromatic hydrocarbon (4 or more rings)	-0.6573	-0.6573
MolWt	*	Molecular Weight Parameter		-0.1325
Const	*	Equation Constant		0.7475
RESULT				Biowin1 (Linear Biodeg Probability) -0.0423

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Polyaromatic hydrocarbon (4 or more rings)	-10.1644	-10.1644
MolWt	*	Molecular Weight Parameter		-3.9527
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	1	Polyaromatic hydrocarbon (4 or more rings)	-0.7993	-0.7993
MolWt	*	Molecular Weight Parameter		-0.6151
Const	*	Equation Constant		3.1992
RESULT				Biowin3 (Survey Model - Ultimate Biodeg) 1.7847

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Polyaromatic hydrocarbon (4 or more rings)	-0.7022	-0.7022
MolWt	*	Molecular Weight Parameter		-0.4016
Const	*	Equation Constant		3.8477
RESULT				Biowin4 (Survey Model - Primary Biodeg) 2.7439

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	14	Aromatic-H	0.0082	0.1151
MolWt	*	Molecular Weight Parameter		-0.8281
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		-0.0009

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	14	Aromatic-H	0.1201	1.6820
MolWt	*	Molecular Weight Parameter		-8.0358
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.0213

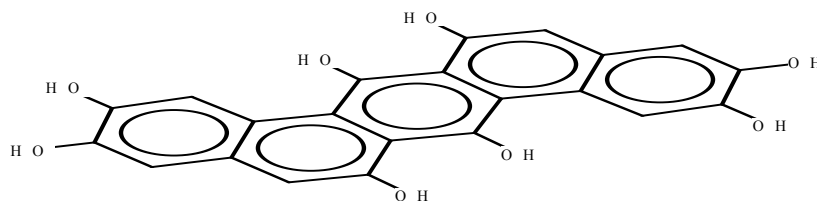
A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Polyaromatic hydrocarbon (4 or more rings)	0.0000	0.0000
Frag	14	Aromatic-H	-0.0954	-1.3360
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		-0.4999

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 ≥ 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 : Oc1cc2c(cc1O)cc(O)c3c(O)c4c5c(cc(O)c(O)c5)cc(O)c4c(O)c32
 CHEM :
 MOL FOR: C22 H14 O8
 MOL WT : 406.35

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

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

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag	8	Aromatic alcohol [-OH]	0.1158	0.9265	
Frag	1	Polyaromatic hydrocarbon (4 or more rings)	-0.6573	-0.6573	
MolWt	*	Molecular Weight Parameter		-0.1935	
Const	*	Equation Constant		0.7475	
RESULT				Biowin1 (Linear Biodeg Probability)	0.8233

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag	8	Aromatic alcohol [-OH]	0.9086	7.2688	
Frag	1	Polyaromatic hydrocarbon (4 or more rings)	-10.1644	-10.1644	
MolWt	*	Molecular Weight Parameter		-5.7702	
RESULT				Biowin2 (Non-Linear Biodeg Probability)	0.0035

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	8	Aromatic alcohol [-OH]	0.0564	0.4510	
Frag	1	Polyaromatic hydrocarbon (4 or more rings)	-0.7993	-0.7993	
MolWt	*	Molecular Weight Parameter		-0.8980	
Const	*	Equation Constant		3.1992	
RESULT				Biowin3 (Survey Model - Ultimate Biodeg)	1.9529

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	8	Aromatic alcohol [-OH]	0.0397	0.3175
Frag	1	Polyaromatic hydrocarbon (4 or more rings)	-0.7022	-0.7022

MolWt	*	Molecular Weight Parameter		-0.5863
Const	*	Equation Constant		3.8477
=====				
RESULT		Biowin4 (Survey Model - Primary Biodeg)		2.8768
=====				

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	8	Aromatic alcohol [-OH]	0.0642	0.5138
Frag	6	Aromatic-H	0.0082	0.0493
MolWt	*	Molecular Weight Parameter		-1.2089
Const	*	Equation Constant		0.7121
=====				
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.0664
=====				

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	8	Aromatic alcohol [-OH]	0.4884	3.9074
Frag	6	Aromatic-H	0.1201	0.7208
MolWt	*	Molecular Weight Parameter		-11.7309
=====				
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.0102
=====				

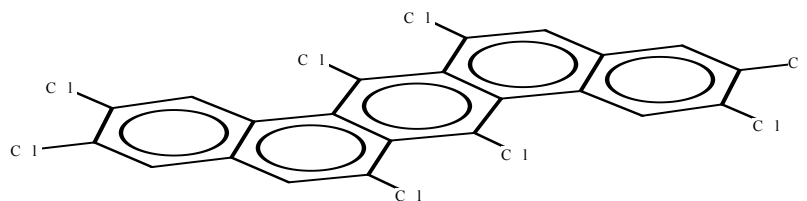
A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	8	Aromatic alcohol [-OH]	0.0807	0.6458
Frag	1	Polyaromatic hydrocarbon (4 or more rings)	0.0000	0.0000
Frag	6	Aromatic-H	-0.0954	-0.5726
Const	*	Equation Constant		0.8361
=====				
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		0.9093
=====				

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 ≥ 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 : Clc1cc2c(cc1Cl)cc(Cl)c3c(Cl)c4c5c(cc(Cl)c(Cl)c5)cc(Cl)c4c(Cl)c32
 CHEM :
 MOL FOR: C22 H6 CL8
 MOL WT : 553.92

----- 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): Recalcitrant
 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	8	Aromatic chloride [-CL]	-0.1824	-1.4594
Frag	1	Polyaromatic hydrocarbon (4 or more rings)	-0.6573	-0.6573
MolWt	*	Molecular Weight Parameter		-0.2637
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		-1.6328

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	8	Aromatic chloride [-CL]	-2.0155	-16.1240
Frag	1	Polyaromatic hydrocarbon (4 or more rings)	-10.1644	-10.1644
MolWt	*	Molecular Weight Parameter		-7.8656
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	8	Aromatic chloride [-CL]	-0.2066	-1.6528
Frag	1	Polyaromatic hydrocarbon (4 or more rings)	-0.7993	-0.7993
MolWt	*	Molecular Weight Parameter		-1.2241
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		-0.4771

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	8	Aromatic chloride [-CL]	-0.1653	-1.3227
Frag	1	Polyaromatic hydrocarbon (4 or more rings)	-0.7022	-0.7022

MolWt	*	Molecular Weight Parameter		-0.7992
Const	*	Equation Constant		3.8477
=====				
RESULT		Biowin4 (Survey Model - Primary Biodeg)		1.0236
=====				

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	8	Aromatic chloride [-CL]	0.0062	0.0494
Frag	6	Aromatic-H	0.0082	0.0493
MolWt	*	Molecular Weight Parameter		-1.6479
Const	*	Equation Constant		0.7121
=====				
RESULT		Biowin5 (MITI Linear Biodeg Probability)		-0.8371
=====				

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	8	Aromatic chloride [-CL]	-0.2191	-1.7532
Frag	6	Aromatic-H	0.1201	0.7208
MolWt	*	Molecular Weight Parameter		-15.9909
=====				
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	8	Aromatic chloride [-CL]	-0.4023	-3.2182
Frag	1	Polyaromatic hydrocarbon (4 or more rings)	0.0000	0.0000
Frag	6	Aromatic-H	-0.0954	-0.5726
Const	*	Equation Constant		0.8361
=====				
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		-2.9547
=====				

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 ≥ 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.