

SMILES : Cc1c(N(=O)(=O))cc(N(=O)(=O))cc1N(=O)(=O)
 CHEM :
 MOL FOR: C7 H5 N3 O6
 MOL WT : 227.13

----- 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	3	Aromatic nitro [-NO2]	-0.3050	-0.9151
Frag	1	Alkyl substituent on aromatic ring	0.0547	0.0547
MolWt	*	Molecular Weight Parameter		-0.1081
Const	*	Equation Constant		0.7475
=====				
RESULT		Biowin1 (Linear Biodeg Probability)		-0.2210
=====				

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Aromatic nitro [-NO2]	-2.5086	-7.5258
Frag	1	Alkyl substituent on aromatic ring	0.5771	0.5771
MolWt	*	Molecular Weight Parameter		-3.2253
=====				
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.0008
=====				

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	3	Aromatic nitro [-NO2]	-0.1696	-0.5088
Frag	1	Alkyl substituent on aromatic ring	-0.0749	-0.0749
MolWt	*	Molecular Weight Parameter		-0.5019
Const	*	Equation Constant		3.1992
=====				
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		2.1136
=====				

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Aromatic nitro [-NO2]	-0.1084	-0.3251
Frag	1	Alkyl substituent on aromatic ring	-0.0685	-0.0685

MolWt	*	Molecular Weight Parameter		-0.3277
Const	*	Equation Constant		3.8477
=====				
RESULT		Biowin4 (Survey Model - Primary Biodeg)		3.1264
=====				

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	3	Aromatic nitro [-NO2]	-0.1876	-0.5628
Frag	1	Aromatic-CH3	0.0415	0.0415
Frag	2	Aromatic-H	0.0082	0.0164
MolWt	*	Molecular Weight Parameter		-0.6757
Const	*	Equation Constant		0.7121
=====				
RESULT		Biowin5 (MITI Linear Biodeg Probability)		-0.4685
=====				

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Aromatic nitro [-NO2]	-2.4035	-7.2104
Frag	1	Aromatic-CH3	0.3072	0.3072
Frag	2	Aromatic-H	0.1201	0.2403
MolWt	*	Molecular Weight Parameter		-6.5571
=====				
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.0000
=====				

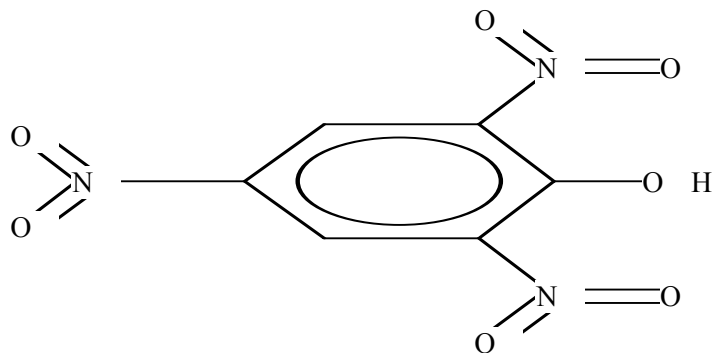
A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Aromatic nitro [-NO2]	-0.2141	-0.6422
Frag	1	Alkyl substituent on aromatic ring	-0.1145	-0.1145
Frag	1	Aromatic-CH3	-0.2573	-0.2573
Frag	2	Aromatic-H	-0.0954	-0.1909
Const	*	Equation Constant		0.8361
=====				
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		-0.3687
=====				

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 : Oc1c(N(=O)(=O))cc(N(=O)(=O))cc1N(=O)(=O)
 CHEM :
 MOL FOR: C6 H3 N3 O7
 MOL WT : 229.11

----- 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	Aromatic alcohol [-OH]	0.1158	0.1158
Frag	3	Aromatic nitro [-NO2]	-0.3050	-0.9151
MolWt	*	Molecular Weight Parameter		-0.1091
Const	*	Equation Constant		0.7475
=====				
RESULT		Biowin1 (Linear Biodeg Probability)		-0.1608
=====				

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.9086	0.9086
Frag	3	Aromatic nitro [-NO2]	-2.5086	-7.5258
MolWt	*	Molecular Weight Parameter		-3.2533
=====				
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.0010
=====				

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	Aromatic alcohol [-OH]	0.0564	0.0564
Frag	3	Aromatic nitro [-NO2]	-0.1696	-0.5088
MolWt	*	Molecular Weight Parameter		-0.5063
Const	*	Equation Constant		3.1992
=====				
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		2.2405
=====				

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.0397	0.0397
Frag	3	Aromatic nitro [-NO2]	-0.1084	-0.3251

MolWt	*	Molecular Weight Parameter		-0.3305
Const	*	Equation Constant		3.8477
=====				
RESULT		Biowin4 (Survey Model - Primary Biodeg)		3.2317
=====				

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	1	Aromatic alcohol [-OH]	0.0642	0.0642
Frag	3	Aromatic nitro [-NO2]	-0.1876	-0.5628
Frag	2	Aromatic-H	0.0082	0.0164
MolWt	*	Molecular Weight Parameter		-0.6816
Const	*	Equation Constant		0.7121
=====				
RESULT		Biowin5 (MITI Linear Biodeg Probability)		-0.4516
=====				

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.4884	0.4884
Frag	3	Aromatic nitro [-NO2]	-2.4035	-7.2104
Frag	2	Aromatic-H	0.1201	0.2403
MolWt	*	Molecular Weight Parameter		-6.6140
=====				
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.0000
=====				

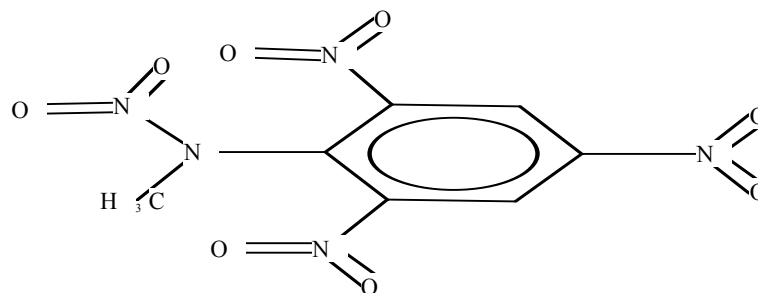
A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.0807	0.0807
Frag	3	Aromatic nitro [-NO2]	-0.2141	-0.6422
Frag	2	Aromatic-H	-0.0954	-0.1909
Const	*	Equation Constant		0.8361
=====				
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		0.0837
=====				

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 : N(=O) (=O) (c1cc (N(=O) (=O)) c (N(N(=O) (=O)) C) c (N(=O) (=O)) c1)
 CHEM :
 MOL FOR: C7 H5 N5 O8
 MOL WT : 287.15

----- 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	3	Aromatic nitro [-NO2]	-0.3050	-0.9151
MolWt	*	Molecular Weight Parameter		-0.1367
Const	*	Equation Constant		0.7475
=====				
RESULT		Biowin1 (Linear Biodeg Probability)		-0.3043
=====				

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Aromatic nitro [-NO2]	-2.5086	-7.5258
MolWt	*	Molecular Weight Parameter		-4.0775
=====				
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.0002
=====				

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	3	Aromatic nitro [-NO2]	-0.1696	-0.5088
MolWt	*	Molecular Weight Parameter		-0.6346
Const	*	Equation Constant		3.1992
=====				
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		2.0558
=====				

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Aromatic nitro [-NO2]	-0.1084	-0.3251
MolWt	*	Molecular Weight Parameter		-0.4143
Const	*	Equation Constant		3.8477
=====				
RESULT		Biowin4 (Survey Model - Primary Biodeg)		3.1083
=====				

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	3	Aromatic nitro [-NO2]	-0.1876	-0.5628
Frag	2	Aromatic-H	0.0082	0.0164
Frag	1	Methyl [-CH3]	0.0004	0.0004
MolWt	*	Molecular Weight Parameter		-0.8543
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		-0.6880

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Aromatic nitro [-NO2]	-2.4035	-7.2104
Frag	2	Aromatic-H	0.1201	0.2403
Frag	1	Methyl [-CH3]	0.0194	0.0194
MolWt	*	Molecular Weight Parameter		-8.2896
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.0000

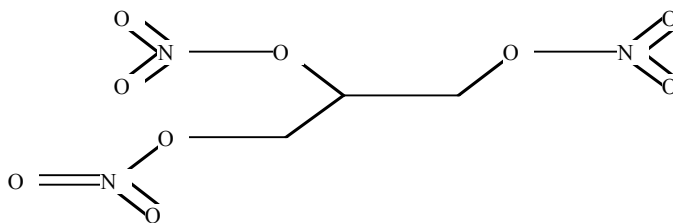
A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Aromatic nitro [-NO2]	-0.2141	-0.6422
Frag	2	Aromatic-H	-0.0954	-0.1909
Frag	1	Methyl [-CH3]	-0.0796	-0.0796
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		-0.0765

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 : O(N(=O)=O)CC(CO(N(=O)=O))O(N(=O)=O)
 CHEM :
 MOL FOR: C3 H5 N3 O9
 MOL WT : 227.09

----- 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): Biodegrades Fast
 Ready Biodegradability Prediction: NO

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
MolWt	*	Molecular Weight Parameter		-0.1081
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		0.6394

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
MolWt	*	Molecular Weight Parameter		-3.2246
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.4462

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
MolWt	*	Molecular Weight Parameter		-0.5018
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		2.6973

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
MolWt	*	Molecular Weight Parameter		-0.3276
Const	*	Equation Constant		3.8477
RESULT		Biowin4 (Survey Model - Primary Biodeg)		3.5201

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	-CH2- [linear]	0.0494	0.0988
Frag	1	-CH- [linear]	-0.0507	-0.0507
MolWt	*	Molecular Weight Parameter		-0.6756
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.0847

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH2- [linear]	0.4295	0.8590
Frag	1	-CH- [linear]	-0.0998	-0.0998
MolWt	*	Molecular Weight Parameter		-6.5557
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.0366

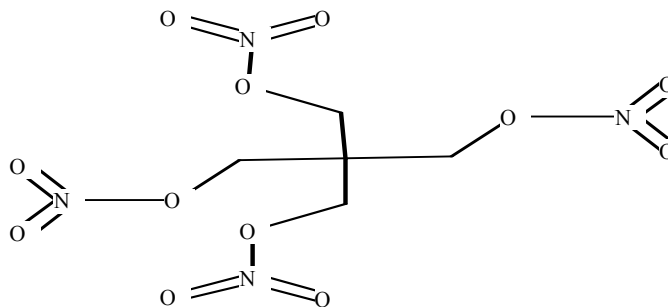
A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH2- [linear]	0.0260	0.0520
Frag	1	-CH- [linear]	-0.1659	-0.1659
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		0.7222

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 : O(N(=O)=O)CC(CO(N(=O)=O))(CO(N(=O)=O))CO(N(=O)=O)
 CHEM :
 MOL FOR: C5 H8 N4 O12
 MOL WT : 316.14

----- 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): Weeks-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	1	Carbon with 4 single bonds & no hydrogens	-0.1839	-0.1839
MolWt	*	Molecular Weight Parameter		-0.1505
Const	*	Equation Constant		0.7475
RESULT				0.4131

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Carbon with 4 single bonds & no hydrogens	-1.7232	-1.7232
MolWt	*	Molecular Weight Parameter		-4.4892
RESULT				0.0390

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	Carbon with 4 single bonds & no hydrogens	-0.2121	-0.2121
MolWt	*	Molecular Weight Parameter		-0.6986
Const	*	Equation Constant		3.1992
RESULT				2.2884

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.1534	-0.1534
MolWt	*	Molecular Weight Parameter		-0.4561
Const	*	Equation Constant		3.8477
RESULT				3.2382

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	1	Carbon with 4 single bonds & no hydrogens	0.0676	0.0676
Frag	4	-CH2- [linear]	0.0494	0.1977
MolWt	*	Molecular Weight Parameter		-0.9405
Const	*	Equation Constant		0.7121
RESULT			Biowin5 (MITI Linear Biodeg Probability)	0.0369

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Carbon with 4 single bonds & no hydrogens	0.3990	0.3990
Frag	4	-CH2- [linear]	0.4295	1.7180
MolWt	*	Molecular Weight Parameter		-9.1265
RESULT			Biowin6 (MITI Non-Linear Biodeg Probability)	0.0112

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	Carbon with 4 single bonds & no hydrogens	-0.3342	-0.3342
Frag	4	-CH2- [linear]	0.0260	0.1040
Const	*	Equation Constant		0.8361
RESULT			Biowin7 (Anaerobic Linear Biodeg Prob)	0.6058

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.