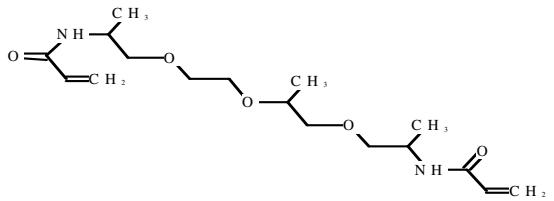

SMILES : O=C(NC(C)COCCOC(C)COCC(C)NC(=O)C=C)C=C
CHEM :
MOL FOR: C17 H30 N2 O5
MOL WT : 342.44

---------- 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): 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	Amide [-C(=O)-N or -C(=S)-N]	0.2102	0.4203
Frag	3	Aliphatic ether [C-O-C]	-0.3474	-1.0421
MolWt	*	Molecular Weight Parameter		-0.1630
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		-0.0373

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Amide [-C(=O)-N or -C(=S)-N]	2.6913	5.3826
Frag	3	Aliphatic ether [C-O-C]	-3.4294	-10.2882
MolWt	*	Molecular Weight Parameter		-4.8626
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.0012

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	Amide [-C(=O)-N or -C(=S)-N]	-0.0542	-0.1084
Frag	3	Aliphatic ether [C-O-C]	-0.0087	-0.0260
MolWt	*	Molecular Weight Parameter		-0.7567
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		2.3080

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Amide [-C(=O)-N or -C(=S)-N]	0.2054	0.4109
Frag	3	Aliphatic ether [C-O-C]	-0.0097	-0.0292
MolWt	*	Molecular Weight Parameter		-0.4941
Const	*	Equation Constant		3.8477

RESULT	Biowin4 (Survey Model - Primary Biodeg)		3.7353

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	Amide [-C(=O)-N or -C(=S)-N]	0.1266	0.2533
Frag	3	Aliphatic ether [C-O-C]	0.0015	0.0044
Frag	3	Methyl [-CH3]	0.0004	0.0012
Frag	5	-CH2- [linear]	0.0494	0.2471
Frag	3	-CH- [linear]	-0.0507	-0.1520
Frag	6	-C=CH [alkenyl hydrogen]	0.0062	0.0371
MolWt	*	Molecular Weight Parameter		-1.0188
Const	*	Equation Constant		0.7121
RESULT	Biowin5 (MITI Linear Biodeg Probability)			0.0845

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Amide [-C(=O)-N or -C(=S)-N]	0.8859	1.7717
Frag	3	Aliphatic ether [C-O-C]	-0.1071	-0.3214
Frag	3	Methyl [-CH3]	0.0194	0.0583
Frag	5	-CH2- [linear]	0.4295	2.1475
Frag	3	-CH- [linear]	-0.0998	-0.2993
Frag	6	-C=CH [alkenyl hydrogen]	0.0285	0.1711
MolWt	*	Molecular Weight Parameter		-9.8858
RESULT	Biowin6 (MITI Non-Linear Biodeg Probability)			0.0212

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	Amide [-C(=O)-N or -C(=S)-N]	-0.5679	-1.1358
Frag	3	Aliphatic ether [C-O-C]	-0.2573	-0.7718
Frag	3	Methyl [-CH3]	-0.0796	-0.2387
Frag	5	-CH2- [linear]	0.0260	0.1299
Frag	3	-CH- [linear]	-0.1659	-0.4976
Frag	6	-C=CH [alkenyl hydrogen]	-0.0735	-0.4411
Const	*	Equation Constant		0.8361
RESULT	Biowin7 (Anaerobic Linear Biodeg Prob)			-2.1189

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.