Fenpropathrin

Other names:	(.+/-.)-Fenpropathrin
	2,2,3,3-Tetramethylcyclopropanecarboxylic acid, cyano(3-phenoxyphenyl)methyl ester (fenpropathrin)
	Cyano(3-phenoxyphenyl)methyl 2,2,3,3-tetramethylcyclopropanecarboxylate
	Cyclopropanecarboxylic acid, 2,2,3,3-tetramethyl-, cyano(3-phenoxyphenyl)methyl ester
	Danimen
	Danitol
	Danitol Fiori
	Danitrol
	Fenpropanate
	Fenpropathrine
	Herald
	Kilumal
	Meiothrin
	Meothrin
	Miothrin
	Ortho danitol
	Rody
	S 3206
	SD 41706
	Smash
	Tame
	WL 41706
	XE-938
	«alpha»-Cyano-3-phenoxybenzyl 2,2,3,3-tetramethyl-1-cyclopropanecarboxylate
	«alpha»-Cyano-3-phenoxybenzyl 2,2,3,3-tetramethylcyclopropanecarboxylate
	Â«alphaÂ»-Cyano-3-phenoxybenzyl 2,2,3,3-tetramethyl-1-cyclopropanecarboxylate
	Ã«alphaÃ»-Cyano-3-phenoxybenzyl 2,2,3,3-tetramethylcyclopropanecarboxylate
Inchi:	InChI=1S/C22H23NO3/c1-21(2)19(22(21,3)4)20(24)26-18(14-23)15-9-8-12-17(13-15)25-
InchiKey:	XQUXKZZNEFRCAW-UHFFFAOYSA-N
Formula:	C22H23NO3
SMILES:	CC1(C)C(C(=O)OC(C#N)c2cccc(Oc3ccccc3)c2)C1(C)C
Mol. weight [g/mol]:	349.42
CAS:	39515-41-8

Physical Properties

Property code	Value	Unit	Source

gf	175.72	kJ/mol	Joback Method
hf	-190.64	kJ/mol	Joback Method
hfus	30.07	kJ/mol	Joback Method
hvap	88.43	kJ/mol	Joback Method
log10ws	-6.03		Estimated Solubility Method
log10ws	-6.03		Aqueous Solubility Prediction Method
logp	5.269		Crippen Method
mcvol	277.150	ml/mol	McGowan Method
pc	1578.46	kPa	Joback Method
rinpol	2498.00		NIST Webbook
rinpol	2498.00		NIST Webbook
rinpol	2514.00		NIST Webbook
rinpol	2495.00		NIST Webbook
tb	959.33	K	Joback Method
tc	1208.31	K	Joback Method
tf	604.70	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.33	J/mol×K	1166.81	Joback Method
cpg	902.40	J/mol×K	959.33	Joback Method
cpg	925.46	J/mol×K	1000.83	Joback Method
cpg	949.54	J/mol×K	1042.32	Joback Method
cpg	974.99	J/mol×K	1083.82	Joback Method
cpg	1002.14	J/mol×K	1125.32	Joback Method
cpg	1062.91	J/mol×K	1208.31	Joback Method
hfust	18.57	kJ/mol	322.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C39515418&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume