Phenothrin

Other names:	2,2-Dimethyl-3-(2-methyl-1-propenyl)cyclopropanecarboxylic acid (3-phenoxy-phenyl)methyl ester 2,2-Dimethyl-3-(2-methylpropenyl)cyclopropanecarboxylic acid m-phenoxybenzyl ester 2,2-Dimethyl-3-(2-methylpropenyl-1)cyclopropancarbonic acid, 3-phenoxybenzyl ester 3-Phenoxybenzyl chrysanthemate 3-phenoxybenzyl 2-dimethyl-3-(methylpropenyl)cyclopropanecarboxylate Anchimanaito 20S Benzyl alcohol, m-phenoxy-, 2,2-dimethyl-3-(2-methylpropenyl)cyclopropanecarboxylate Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, (3-phenoxyphenyl)methyl ester Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, m-phenoxybenzyl ester Cyclopropanecarboxylic acid,2,2-dimethyl-3-(2-methylpropen-1-yl), 3-phenoxybenzyl ester Duet Fenothrin Fenotrina Multicide 2154 OMS 1809 OMS 1810 PT 515 Phenothrin, isomer 1 Phenothrin, isomer 2 Phenothrine Phenoxythrin Phonothrin Pibutin S 2539 S 2539 (pesticide) Solo Solo (insecticide) Sumithrin Sumitrin m-Phenoxybenzyl 2,2-dimethyl-3-(2-methylpropenyl)cyclopropanecarboxylate
Inchi:	InChI=1S/C23H26O3/c1-16(2)13-20-21(23(20,3)4)22(24)25-15-17-9-8-12-19(14-17)26-18
InchiKey:	SBNFWQZLDJGRLK-UHFFFAOYSA-N
Formula:	C23H26O3
SMILES:	CC(C)=CC1C(C(=O)OCc2cccc(Oc3ccccc3)c2)C1(C)C
Mol. weight [g/mol]:	350.45
CAS:	26002-80-2

Physical Properties

Property code	Value	Unit	Source
gf	130.56	kJ/mol	Joback Method
hf	-278.69	kJ/mol	Joback Method
hfus	39.87	kJ/mol	Joback Method
hvap	81.75	kJ/mol	Joback Method
log10ws	-5.24		Aqueous Solubility Prediction Method
log10ws	-5.24		Estimated Solubility Method
logp	5.761		Crippen Method
mcvol	285.560	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinpol	2531.00		NIST Webbook
rinpol	2545.00		NIST Webbook
rinpol	2531.00		NIST Webbook
tb	884.37	K	Joback Method
tc	1120.38	K	Joback Method
tf	523.04	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	903.83	J/mol×K	884.37	Joback Method
cpg	923.82	J/mol×K	923.70	Joback Method
cpg	943.32	J/mol×K	963.04	Joback Method
cpg	962.54	J/mol×K	1002.37	Joback Method
cpg	981.67	J/mol×K	1041.71	Joback Method
cpg	1000.93	J/mol×K	1081.04	Joback Method
cpg	1020.52	J/mol×K	1120.38	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26002802&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

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
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