Methoprene

Other names:	(2E,4E)-3,7,11-Trimethyl-11-methoxydodeca-2,4-dienoic acid 1-methylethyl ester 2,4-Dodecadienoic acid, 11-methoxy-3,7,11-trimethyl-, 1-methylethyl ester, (2E,4E)- 2,4-Dodecadienoic acid, 11-methoxy-3,7,11-trimethyl-, 1-methylethyl ester, (E,E)- Altosid Altosid IGR Altosid Liquid Larvicide Altosid SR 10 Altoside Apex Apex (pesticide) Bioprene BM Fire Ant Killer Bait Diacon Dianex ENT 70460 Isopropyl (2E,4E)-11-methoxy-3,7,11-trimethyl-2,4-dodecadienoate Juvemon Kabat Manta Manta (hormone) Methoprene S Minex OMS 1697 Pharoid Precor Starbar Inhibitor ZPA 1019 ZR 515 dl-Isopropyl 11-methoxy-3,7,11-trimethyl-trans-trans-2,4-dodecadienoate isopropyl (2E,4E)-11-methoxy-3,7,11-trimethyldodeca-2,4-dienoate
Inchi:	InChI=1S/C19H34O3/c1-15(2)22-18(20)14-17(4)11-8-10-16(3)12-9-13-19(5,6)21-7/h8,11
InchiKey:	NFGXHKASABOEEW-LDRANXPESA-N
Formula:	C19H34O3
SMILES:	COC(C)(C)CCCC(C)CC=CC(C)=CC(=O)OC(C)C
Mol. weight [g/mol]:	310.47
CAS:	40596-69-8

Physical Properties

Property code	Value	Unit	Source
gf	-79.97	kJ/mol	Joback Method
hf	-607.17	kJ/mol	Joback Method
hfus	33.57	kJ/mol	Joback Method
hvap	67.38	kJ/mol	Joback Method
log10ws	-5.19		Estimated Solubility Method
log10ws	-5.19		Aqueous Solubility Prediction Method
logp	5.062		Crippen Method
mcvol	283.280	ml/mol	McGowan Method
pc	1214.90	kPa	Joback Method
rinpol	2097.00		NIST Webbook
rinpol	2097.00		NIST Webbook
tb	736.92	K	Joback Method
tc	926.61	K	Joback Method
tf	346.58	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.01	J/mol×K	736.92	Joback Method
cpg	855.93	J/mol×K	768.54	Joback Method
cpg	873.84	J/mol×K	800.15	Joback Method
cpg	890.77	J/mol×K	831.77	Joback Method
cpg	906.79	J/mol×K	863.38	Joback Method
cpg	921.95	J/mol×K	895.00	Joback Method
cpg	936.28	J/mol×K	926.61	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40596698&Units=SI

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

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

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