Allethrin, isomers 1,2

Inchi: InChI=1S/C19H26O3/c1-7-8-13-12(4)16(10-15(13)20)22-18(21)17-14(9-11(2)3)19(17,5)6
InchiKey: ZCVAOQKBXKSDMS-UHFFFAOYSA-N
Formula: C19H26O3
SMILES: C=CCC1=C(C)C(OC(=O)C2C(C=C(C)C)C2(C)C)CC1=O
Mol. weight [g/mol]: 302.41

Physical Properties

Property code	Value	Unit	Source
gf	-0.81	kJ/mol	Joback Method
hf	-442.45	kJ/mol	Joback Method
hfus	33.23	kJ/mol	Joback Method
hvap	70.68	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.002		Crippen Method
mcvol	252.960	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinpol	2066.00		NIST Webbook
tb	800.99	K	Joback Method
tc	1021.94	K	Joback Method
tf	493.53	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.44	J/mol×K	800.99	Joback Method
cpg	812.32	J/mol×K	837.82	Joback Method
cpg	831.48	J/mol×K	874.64	Joback Method
cpg	850.06	J/mol×K	911.47	Joback Method
cpg	868.19	J/mol×K	948.29	Joback Method
cpg	886.00	J/mol×K	985.12	Joback Method
cpg	903.63	J/mol×K	1021.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R566308&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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