

Tefluthrin

Other names:	Tetrafluthrin
Inchi:	InChI=1S/C17H14ClF7O2/c1-6-11(19)13(21)7(14(22)12(6)20)5-27-15(26)10-8(16(10,2)3
InchiKey:	ZFHGXWPMULPQSE-SZGBIDFHSA-N
Formula:	C17H14ClF7O2
SMILES:	<chem>Cc1c(F)c(F)c(COC(=O)C2C(C=C(Cl)C(F)(F)F)C2(C)C)c(F)c1F</chem>
Mol. weight [g/mol]:	418.73
CAS:	93907-48-3

Physical Properties

Property code	Value	Unit	Source
gf	-1338.65	kJ/mol	Joback Method
hf	-1702.30	kJ/mol	Joback Method
hfus	45.88	kJ/mol	Joback Method
hvap	63.73	kJ/mol	Joback Method
log10ws	-7.32		Aqueous Solubility Prediction Method
log10ws	-7.32		Estimated Solubility Method
logp	5.552		Crippen Method
mcvol	243.540	ml/mol	McGowan Method
pc	1356.63	kPa	Joback Method
rinpol	1816.00		NIST Webbook
rinpol	1816.00		NIST Webbook
rinpol	1826.00		NIST Webbook
rinpol	1821.00		NIST Webbook
tb	747.00	K	Joback Method
tc	934.66	K	Joback Method
tf	317.75	K	Aqueous Solubility Prediction Method
vc	1.002	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.60	J/mol×K	747.00	Joback Method

cpg	712.87	J/mol×K	778.28	Joback Method
cpg	725.66	J/mol×K	809.55	Joback Method
cpg	738.06	J/mol×K	840.83	Joback Method
cpg	750.19	J/mol×K	872.10	Joback Method
cpg	762.13	J/mol×K	903.38	Joback Method
cpg	773.99	J/mol×K	934.66	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=C93907483&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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