

Cypermethrin, isomer 3

Inchi:	InChI=1S/C23H21Cl2NO3/c1-23(2)19(12-20(24)25)21(23)22(27)28-14-16(13-26)15-7-6-
InchiKey:	IHURASJUKICJC-UHFFFAOYSA-N
Formula:	C23H21Cl2NO3
SMILES:	CC1(C)C(C=C(Cl)Cl)C1C(=O)OCC(C#N)c1cccc(Oc2cccc2)c1
Mol. weight [g/mol]:	430.32

Physical Properties

Property code	Value	Unit	Source
gf	237.44	kJ/mol	Joback Method
hf	-150.57	kJ/mol	Joback Method
hfus	46.24	kJ/mol	Joback Method
hvap	100.61	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	6.220		Crippen Method
mcvol	311.420	ml/mol	McGowan Method
pc	1397.50	kPa	Joback Method
rinpol	2850.00		NIST Webbook
rinpol	2845.00		NIST Webbook
rinpol	2850.00		NIST Webbook
tb	1060.87	K	Joback Method
tc	1317.23	K	Joback Method
tf	632.87	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	982.34	J/molxK	1060.87	Joback Method
cpg	1001.95	J/molxK	1103.60	Joback Method
cpg	1022.17	J/molxK	1146.32	Joback Method
cpg	1043.27	J/molxK	1189.05	Joback Method
cpg	1065.53	J/molxK	1231.78	Joback Method
cpg	1089.19	J/molxK	1274.50	Joback Method
cpg	1114.54	J/molxK	1317.23	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R566115&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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