Cyhalothrin, isomer 1

Inchi: InChI=1S/C23H19ClF3NO3/c1-22(2)17(12-19(24)23(25,26)27)20(22)21(29)31-18(13-28)
InchiKey: ZXQYGBMAQZUVMI-UNOMPAQXSA-N
Formula: C23H19ClF3NO3
SMILES: CC1(C)C(C=C(Cl)C(F)(F)F)C1C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 449.85

Physical Properties

Property code	Value	Unit	Source
gf	-332.22	kJ/mol	Joback Method
hf	-731.91	kJ/mol	Joback Method
hfus	43.87	kJ/mol	Joback Method
hvap	92.48	kJ/mol	Joback Method
log10ws	-7.20		Crippen Method
logp	6.544		Crippen Method
mcvol	304.490	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	2574.00		NIST Webbook
rinpol	2572.00		NIST Webbook
tb	1018.02	K	Joback Method
tc	1260.66	K	Joback Method
tf	607.14	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.31	J/mol×K	1018.02	Joback Method
cpg	995.35	J/mol×K	1058.46	Joback Method
cpg	1013.87	J/mol×K	1098.90	Joback Method
cpg	1033.11	J/mol×K	1139.34	Joback Method
cpg	1053.34	J/mol×K	1179.78	Joback Method
cpg	1074.81	J/mol×K	1220.22	Joback Method
cpg	1097.78	J/mol×K	1260.66	Joback Method

Sources

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=R566071&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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