

Cypermethrin

Other names: [cyano-[3-(phenoxy)phenyl]methyl]
Inchi: 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropane-1-carboxylate
InchiKey: KAATUXNTWXVJKI-UHFFFAOYSA-N
Formula: C22H19Cl2NO3
SMILES: CC1(C)C(C=C(Cl)Cl)C1C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 416.30
CAS: 52315-07-8

Physical Properties

Property code	Value	Unit	Source
gf	229.02	kJ/mol	Joback Method
hf	-129.93	kJ/mol	Joback Method
hfus	43.65	kJ/mol	Joback Method
hvap	98.39	kJ/mol	Joback Method
log10ws	-8.02		Estimated Solubility Method
log10ws	-8.02		Aqueous Solubility Prediction Method
logp	6.178		Crippen Method
mcvol	297.330	ml/mol	McGowan Method
pc	1503.48	kPa	Joback Method
rinpol	2815.00		NIST Webbook
rinpol	2784.00		NIST Webbook
rinpol	2815.00		NIST Webbook
rinpol	2755.00		NIST Webbook
rinpol	2825.00		NIST Webbook
tb	1037.99	K	Joback Method
tc	1295.90	K	Joback Method
tf	351.27	K	Aqueous Solubility Prediction Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	919.60	J/mol×K	1037.99	Joback Method
cpg	938.26	J/mol×K	1080.97	Joback Method
cpg	957.45	J/mol×K	1123.96	Joback Method
cpg	977.45	J/mol×K	1166.94	Joback Method
cpg	998.51	J/mol×K	1209.93	Joback Method
cpg	1020.91	J/mol×K	1252.91	Joback Method
cpg	1044.92	J/mol×K	1295.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52315078&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
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

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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