CYPERMETHRIN

Other names: [cyano-[3-(phenoxy)phenyl]methyl] 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropane-1-carboxylate

Inchi: InChI=1S/C22H19Cl2NO3/c1-22(2)17(12-19(23)24)20(22)21(26)28-18(13-25)14-7-6-10-1

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

Physical Properties

Property code	Value	Unit	Source
hfus	43.65	kJ/mol	Joback Method
log10ws	-8.02		Aqueous Solubility Prediction Method
log10ws	-8.02		Estimated Solubility Method
logp	6.178		Crippen Method
mcvol	297.330	ml/mol	McGowan Method
rinpol	2755.00		NIST Webbook
rinpol	2815.00		NIST Webbook
rinpol	2784.00		NIST Webbook
rinpol	2825.00		NIST Webbook
rinpol	2815.00		NIST Webbook
tf	351.27	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52315078&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point