CYFLUTHRIN

Other names:

BAY-FCR 1272
BAY-VI 1704
Baythroid
Baythroid H
Beta-cyfluthrin
Bulldock
Cyano(4-fluoro-3-phenoxyphenyl)methyl 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropanecarboxylate
Cyclopropanecarboxylic acid, 2-(2,2-dichlorovinyl)-3,3-dimethyl-, ester with (4-fluoro-3-phenoxyphenyl)hydroxyacetonitrile
Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(4-fluoro-3-phenoxyphenyl)methyl ester
Cyfluthin
Cyfluthine
Cyfoxylate
Eulan SP
FCR 1272
FCR 4545
Responsar
Sofac
Solfac
Syfrutrin
Tempo 2
[cyano-[4-fluoro-3-(phenoxy)phenyl]methyl] 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropane-1-carboxylate
«alpha»-cyano-4-fluoro-3-phenoxybenzyl 3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate
«beta»-Cyfluthrin

Inchi: InChI=1S/C22H18Cl2FNO3/c1-22(2)15(11-19(23)24)20(22)21(27)29-18(12-26)13-8-9-16

InchiKey: QQODLKZGRKWIFG-UHFFFAOYSA-N

Formula: C22H18Cl2FNO3

SMILES: CC1(C)C(C=C(Cl)Cl)C1C(=O)OC(C#N)c1ccc(F)c(Oc2ccccc2)c1

Mol. weight [g/mol]: 434.29

Physical Properties

Property code	Value	Unit	Source
hfus	46.34	kJ/mol	Joback Method
log10ws	-7.34		Aqueous Solubility Prediction Method
log10ws	-7.34		Estimated Solubility Method
logp	6.317		Crippen Method

mcvol	299.100	ml/mol	McGowan Method
tf	384.92	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	925.27	J/mol×K	1042.24	Joback Method
cpg	943.33	J/mol×K	1084.31	Joback Method
cpg	961.89	J/mol×K	1126.39	Joback Method
cpg	981.18	J/mol×K	1168.46	Joback Method
cpg	1001.44	J/mol×K	1210.54	Joback Method
cpg	1022.92	J/mol×K	1252.61	Joback Method
cpg	1045.85	J/mol×K	1294.69	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C68359375&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
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

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
tf: Normal melting (fusion) point

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