Flucythrinate

Other names:	AC 222705
	Benzeneacetic acid, 4-(difluoromethoxy)-«alpha»-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester
	Benzeneacetic acid, 4-(difluoromethoxy)-Â«alphaÂ»-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester
	CyBolt
	Flucythrinate, isomer 1
	Flucythrinate, isomer 2
	Fluorocythrin
	Pay-Off
	[cyano-[3-(phenoxy)phenyl]methyl] 2-[4-(difluoromethoxy)phenyl]-3-methylbutanoate
	cyano(3-phenoxyphenyl)methyl 2-[4-difluoromethoxy)phenyl]-3-methylbutyrate
Inchi:	InChI=1S/C26H23F2NO4/c1-17(2)24(18-11-13-21(14-12-18)32-26(27)28)25(30)33-23(16
InchiKey:	GBIHOLCMZGAKNG-UHFFFAOYSA-N
Formula:	C26H23F2NO4
SMILES:	CC(C)C(C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1)c1ccc(OC(F)F)cc1
Mol. weight [g/mol]:	451.46
CAS:	70124-77-5

Physical Properties

Property code	Value	Unit	Source
gf	-224.11	kJ/mol	Joback Method
hf	-651.02	kJ/mol	Joback Method
hfus	43.18	kJ/mol	Joback Method
hvap	102.89	kJ/mol	Joback Method
log10ws	-6.88		Aqueous Solubility Prediction Method
log10ws	-6.88		Estimated Solubility Method
logp	6.628		Crippen Method
mcvol	330.020	ml/mol	McGowan Method
pc	1255.70	kPa	Joback Method
rinpol	2871.00		NIST Webbook
rinpol	2874.00		NIST Webbook
rinpol	2844.00		NIST Webbook
rinpol	2844.00		NIST Webbook
rinpol	2847.00		NIST Webbook
tb	1104.27	K	Joback Method
tc	1356.15	K	Joback Method

tf	609.87	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1063.85	J/mol×K	1104.27	Joback Method
cpg	1071.79	J/mol×K	1146.25	Joback Method
cpg	1078.03	J/mol×K	1188.23	Joback Method
cpg	1082.64	J/mol×K	1230.21	Joback Method
cpg	1085.69	J/mol×K	1272.19	Joback Method
cpg	1087.24	J/mol×K	1314.17	Joback Method
cpg	1087.37	J/mol×K	1356.15	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C70124775&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/AqueousDa

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