FLUCYTHRINATE

Other names: AC 222705

Benzeneacetic acid, 4-(difluoromethoxy)-«alpha»-(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]: 451.47

Physical Properties

Property code	Value	Unit	Source
hfus	43.18	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
rinpol	2844.00		NIST Webbook
rinpol	2847.00		NIST Webbook
rinpol	2871.00		NIST Webbook
rinpol	2874.00		NIST Webbook
rinpol	2844.00		NIST Webbook
tf	395.99	K	Cheméo Relay (1.0)

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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C70124775&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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