Fluvalinate

Other names: Apistan
DL-Valine, N-[2-chloro-4-(trifluoromethyl)phenyl]-, cyano(3-phenoxyphenyl)methyl ester
Fluvalinate, isomer 1
Fluvalinate, isomer 2
Kartan
Mavrik
Mavrik aquaflow
Minadox
Valine, N-[2-chloro-4-(trifluoromethyl)phenyl]-, cyano(3-phenoxyphenyl)methyl ester
ZR 3210
[cyano-[3-(phenoxy)phenyl]methyl] 2-[[2-chloro-4-(trifluoromethyl)phenyl]amino]-3-methylbutanoate

Inchi: InChI=1S/C26H22ClF3N2O3/c1-16(2)24(32-22-12-11-18(14-21(22)27)26(28,29)30)25(33

InchiKey: INISTDXBRIBGOC-UHFFFAOYSA-N

Formula: C26H22ClF3N2O3

SMILES: CC(C)C(Nc1ccc(C(F)(F)F)cc1Cl)C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]: 502.91

CAS: 69409-94-5

Physical Properties

Property code	Value	Unit	Source
gf	-240.81	kJ/mol	Joback Method
hf	-692.12	kJ/mol	Joback Method
hfus	50.09	kJ/mol	Joback Method
hvap	110.24	kJ/mol	Joback Method
log10ws	-8.00		Aqueous Solubility Prediction Method
log10ws	-8.00		Estimated Solubility Method
logp	7.396		Crippen Method
mcvol	348.140	ml/mol	McGowan Method
pc	1207.31	kPa	Joback Method
rinpol	2973.00		NIST Webbook
rinpol	2966.00		NIST Webbook
rinpol	2964.00		NIST Webbook
rinpol	2976.00		NIST Webbook
tb	1170.91	K	Joback Method
tc	1434.20	K	Joback Method

tf	700.75	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1111.17	J/mol×K	1170.91	Joback Method
cpg	1118.91	J/mol×K	1214.79	Joback Method
cpg	1125.54	J/mol×K	1258.67	Joback Method
cpg	1131.23	J/mol×K	1302.56	Joback Method
cpg	1136.11	J/mol×K	1346.44	Joback Method
cpg	1140.32	J/mol×K	1390.32	Joback Method
cpg	1144.01	J/mol×K	1434.20	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C69409945&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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