Flumetralin

Other names:	2-Chloro-N-(2,6-dinitro-4-(trifluoromethyl)phenyl)-N-ethyl-6-fluorobenzenemethanamine
	CGA-41065
	Flumetraline
	Prime+
Inchi:	InChI=1S/C16H12ClF4N3O4/c1-2-22(8-10-11(17)4-3-5-12(10)18)15-13(23(25)26)6-9(16
InchiKey:	PWNAWOCHVWERAR-UHFFFAOYSA-N
Formula:	C16H12ClF4N3O4
SMILES:	CCN(Cc1c(F)cccc1Cl)c1c([N+](=O)[O-])cc(C(F)(F)F)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	421.73

Physical Properties

Property code	Value	Unit	Source
hfus	58.18	kJ/mol	Joback Method
log10ws	-6.78		Aqueous Solubility Prediction Method
log10ws	-6.78		Estimated Solubility Method
logp	5.341		Crippen Method
mcvol	252.920	ml/mol	McGowan Method
tb	643.38	K	Cheméo Relay (1.0)
tf	372.31	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.01	J/mol×K	991.14	Joback Method
cpg	768.07	J/mol×K	1032.04	Joback Method
cpg	776.41	J/mol×K	1072.95	Joback Method
cpg	784.15	J/mol×K	1113.85	Joback Method
cpg	791.40	J/mol×K	1154.75	Joback Method
cpg	798.28	J/mol×K	1195.66	Joback Method
cpg	804.91	J/mol×K	1236.56	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=C62924703&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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point