Fluometuron, HFBA

Inchi: InChI=1S/C14H10F10N2O2/c1-25(2)10(28)26(8-5-3-7(4-6-8)12(17,18)19)9(27)11(15,16)
InchiKey: PNNDBKHPFIDXDY-UHFFFAOYSA-N
Formula: C14H10F10N2O2
SMILES: CN(C)C(=O)N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 428.23

Physical Properties

Property code	Value	Unit	Source
gf	-1803.24	kJ/mol	Joback Method
hf	-2193.43	kJ/mol	Joback Method
hfus	36.05	kJ/mol	Joback Method
hvap	53.92	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.553		Crippen Method
mcvol	225.160	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
rinpol	1718.00		NIST Webbook
rinpol	1718.00		NIST Webbook
tb	663.78	K	Joback Method
tc	834.21	K	Joback Method
tf	466.86	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.70	J/mol×K	663.78	Joback Method
cpg	667.49	J/mol×K	692.19	Joback Method
cpg	678.34	J/mol×K	720.59	Joback Method
cpg	688.31	J/mol×K	749.00	Joback Method
cpg	697.49	J/mol×K	777.40	Joback Method
cpg	705.96	J/mol×K	805.81	Joback Method
cpg	713.79	J/mol×K	834.21	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R220354&Units=SI

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