Metoxuron, HFBA

Inchi: InChI=1S/C14H12ClF7N2O3/c1-23(2)11(26)24(7-4-5-9(27-3)8(15)6-7)10(25)12(16,17)13
InchiKey: XRBBFSDUHNIZDN-UHFFFAOYSA-N
Formula: C14H12ClF7N2O3
SMILES: COc1ccc(N(C(=O)N(C)C)C(=O)C(F)(F)C(F)(F)C(F)(F)F)cc1Cl
Mol. weight [g/mol]: 424.70

Physical Properties

Property code	Value	Unit	Source
gf	-1348.21	kJ/mol	Joback Method
hf	-1755.78	kJ/mol	Joback Method
hfus	39.22	kJ/mol	Joback Method
hvap	65.12	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.196		Crippen Method
mcvol	237.960	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
rinpol	1870.00		NIST Webbook
rinpol	1870.00		NIST Webbook
tb	734.03	K	Joback Method
tc	920.05	K	Joback Method
tf	527.34	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.63	J/mol×K	734.03	Joback Method
cpg	690.74	J/mol×K	765.03	Joback Method
cpg	700.98	J/mol×K	796.04	Joback Method
cpg	710.42	J/mol×K	827.04	Joback Method
cpg	719.13	J/mol×K	858.04	Joback Method
cpg	727.19	J/mol×K	889.04	Joback Method
cpg	734.67	J/mol×K	920.05	Joback Method

Sources

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=R220394&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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