Linuron, HFBA

Inchi: InChI=1S/C13H9Cl2F7N2O3/c1-23(27-2)10(26)24(6-3-4-7(14)8(15)5-6)9(25)11(16,17)12
InchiKey: WQKIYZMNEKUMDR-UHFFFAOYSA-N
Formula: C13H9Cl2F7N2O3
SMILES: CON(C)C(=O)N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)c1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 445.12

Physical Properties

Property code	Value	Unit	Source
gf	-1368.56	kJ/mol	Joback Method
hf	-1750.88	kJ/mol	Joback Method
hfus	40.83	kJ/mol	Joback Method
hvap	67.28	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.772		Crippen Method
mcvol	236.110	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	1775.00		NIST Webbook
rinpol	1775.00		NIST Webbook
tb	748.58	K	Joback Method
tc	939.47	K	Joback Method
tf	545.99	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.55	J/mol×K	748.58	Joback Method
cpg	660.20	J/mol×K	780.39	Joback Method
cpg	669.02	J/mol×K	812.21	Joback Method
cpg	677.10	J/mol×K	844.02	Joback Method
cpg	684.50	J/mol×K	875.84	Joback Method
cpg	691.32	J/mol×K	907.65	Joback Method
cpg	697.61	J/mol×K	939.47	Joback Method

Sources

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=R220374&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