Diuron, HFBA

Inchi: InChI=1S/C13H9Cl2F7N2O2/c1-23(2)10(26)24(6-3-4-7(14)8(15)5-6)9(25)11(16,17)12(18
InchiKey: GTOSHOMNZWCUAY-UHFFFAOYSA-N
Formula: C13H9Cl2F7N2O2
SMILES: CN(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]: 429.12

Physical Properties

Property code	Value	Unit	Source
gf	-1263.56	kJ/mol	Joback Method
hf	-1618.66	kJ/mol	Joback Method
hfus	39.64	kJ/mol	Joback Method
hvap	64.87	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	4.841		Crippen Method
mcvol	230.240	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	1767.00		NIST Webbook
rinpol	1767.00		NIST Webbook
tb	726.16	K	Joback Method
tc	917.12	K	Joback Method
tf	523.76	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.07	J/mol×K	726.16	Joback Method
cpg	635.99	J/mol×K	757.99	Joback Method
cpg	645.06	J/mol×K	789.81	Joback Method
cpg	653.38	J/mol×K	821.64	Joback Method
cpg	661.01	J/mol×K	853.47	Joback Method
cpg	668.06	J/mol×K	885.30	Joback Method
cpg	674.61	J/mol×K	917.12	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=R220309&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