Chlorbromuron, HFBA

Inchi: InChI=1S/C13H9BrClF7N2O3/c1-23(27-2)10(26)24(6-3-4-7(14)8(15)5-6)9(25)11(16,17)1
InchiKey: APQJFUKBFABUNG-UHFFFAOYSA-N
Formula: C13H9BrClF7N2O3
SMILES: CON(C)C(=O)N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)c1ccc(Br)c(Cl)c1
Mol. weight [g/mol]: 489.57

Physical Properties

Property code	Value	Unit	Source
gf	-1342.31	kJ/mol	Joback Method
hf	-1708.81	kJ/mol	Joback Method
hfus	41.92	kJ/mol	Joback Method
hvap	69.33	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.882		Crippen Method
mcvol	241.370	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
rinpol	1856.00		NIST Webbook
rinpol	1856.00		NIST Webbook
tb	777.31	K	Joback Method
tc	974.57	K	Joback Method
tf	575.87	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.98	J/mol×K	777.31	Joback Method
cpg	669.09	J/mol×K	810.19	Joback Method
cpg	677.43	J/mol×K	843.06	Joback Method
cpg	685.07	J/mol×K	875.94	Joback Method
cpg	692.11	J/mol×K	908.81	Joback Method
cpg	698.64	J/mol×K	941.69	Joback Method
cpg	704.75	J/mol×K	974.57	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=R220230&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

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