Chlortoluron, HFBA

Inchi: InChI=1S/C14H12ClF7N2O2/c1-7-4-5-8(6-9(7)15)24(11(26)23(2)3)10(25)12(16,17)13(18
InchiKey: YJWLAPUVCFNLAN-UHFFFAOYSA-N
Formula: C14H12ClF7N2O2
SMILES: Cc1ccc(N(C(=O)N(C)C)C(=O)C(F)(F)C(F)(F)C(F)(F)F)cc1Cl
Mol. weight [g/mol]: 408.70

Physical Properties

Property code	Value	Unit	Source
gf	-1243.21	kJ/mol	Joback Method
hf	-1623.56	kJ/mol	Joback Method
hfus	38.03	kJ/mol	Joback Method
hvap	62.71	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.496		Crippen Method
mcvol	232.090	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	1720.00		NIST Webbook
rinpol	1720.00		NIST Webbook
tb	711.61	K	Joback Method
tc	897.47	K	Joback Method
tf	505.11	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.03	J/mol×K	711.61	Joback Method
cpg	665.45	J/mol×K	742.59	Joback Method
cpg	675.97	J/mol×K	773.56	Joback Method
cpg	685.68	J/mol×K	804.54	Joback Method
cpg	694.65	J/mol×K	835.52	Joback Method
cpg	702.97	J/mol×K	866.49	Joback Method
cpg	710.71	J/mol×K	897.47	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=R220250&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