Zoxamide

Inchi: InChI=1S/C14H16Cl3NO2/c1-4-14(3,12(19)7-15)18-13(20)9-5-10(16)8(2)11(17)6-9/h5-6
InchiKey: SOUGWDPPRBKJEX-UHFFFAOYSA-N
Formula: C14H16Cl3NO2
SMILES: CCC(C)(NC(=O)c1cc(Cl)c(C)c(Cl)c1)C(=O)CCl
Mol. weight [g/mol]: 336.64

Physical Properties

Property code	Value	Unit	Source
gf	-50.88	kJ/mol	Joback Method
hf	-357.83	kJ/mol	Joback Method
hfus	38.36	kJ/mol	Joback Method
hvap	82.81	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.008		Crippen Method
mcvol	234.200	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
rinpol	2428.00		NIST Webbook
tb	828.31	K	Joback Method
tc	1058.48	K	Joback Method
tf	556.22	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.42	J/mol×K	828.31	Joback Method
cpg	622.62	J/mol×K	866.67	Joback Method
cpg	632.95	J/mol×K	905.03	Joback Method
cpg	642.46	J/mol×K	943.40	Joback Method
cpg	651.23	J/mol×K	981.76	Joback Method
cpg	659.33	J/mol×K	1020.12	Joback Method
cpg	666.81	J/mol×K	1058.48	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R566833&Units=SI

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