N-(2-hydroxyethyl) alpha,alpha-dichloropropionamide

Inchi: InChI=1S/C5H9Cl2NO2/c1-5(6,7)4(10)8-2-3-9/h9H,2-3H2,1H3,(H,8,10)
InchiKey: VUMQYOYMVBQYQU-UHFFFAOYSA-N
Formula: C5H9Cl2NO2
SMILES: CC(Cl)(Cl)C(=O)NCCO
Mol. weight [g/mol]: 186.04
CAS: 83704-00-1

Physical Properties

Property code	Value	Unit	Source
gf	-206.15	kJ/mol	Joback Method
hf	-398.10	kJ/mol	Joback Method
hfus	20.47	kJ/mol	Joback Method
hvap	64.06	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.289		Crippen Method
mcvol	123.210	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
tb	581.65	K	Joback Method
tc	777.06	K	Joback Method
tf	371.78	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.61	J/mol×K	581.65	Joback Method
cpg	279.34	J/mol×K	614.22	Joback Method
cpg	286.56	J/mol×K	646.79	Joback Method
cpg	293.29	J/mol×K	679.35	Joback Method
cpg	299.55	J/mol×K	711.92	Joback Method
cpg	305.39	J/mol×K	744.49	Joback Method
cpg	310.84	J/mol×K	777.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C83704001&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume