Acetamide, n-(2,2,2-trichloro-1-hydroxyethyl)-

Inchi: InChI=1S/C4H6Cl3NO2/c1-2(9)8-3(10)4(5,6)7/h3,10H,1H3,(H,8,9)
InchiKey: WVECDRAYBGJMIV-UHFFFAOYSA-N
Formula: C4H6Cl3NO2
SMILES: CC(=O)NC(O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 206.46
CAS: 5445-85-2

Physical Properties

Property code	Value	Unit	Source
gf	-228.94	kJ/mol	Joback Method
hf	-398.48	kJ/mol	Joback Method
hfus	18.56	kJ/mol	Joback Method
hvap	65.83	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	0.811		Crippen Method
mcvol	121.360	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	595.76	K	Joback Method
tc	802.14	K	Joback Method
tf	375.43	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.32	J/mol×K	595.76	Joback Method
cpg	254.57	J/mol×K	630.16	Joback Method
cpg	260.32	J/mol×K	664.55	Joback Method
cpg	265.59	J/mol×K	698.95	Joback Method
cpg	270.43	J/mol×K	733.35	Joback Method
cpg	274.87	J/mol×K	767.74	Joback Method
cpg	278.94	J/mol×K	802.14	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=C5445852&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume