Ethanethioic acid, dichloro-, S-(1-hydroxy-1-methylethyl) ester

Inchi: InChI=1S/C5H8Cl2O2S/c1-5(2,9)10-4(8)3(6)7/h3,9H,1-2H3
InchiKey: VTFPEDMFUNDKGF-UHFFFAOYSA-N
Formula: C5H8Cl2O2S
SMILES: CC(C)(O)SC(=O)C(Cl)Cl
Mol. weight [g/mol]: 203.09
CAS: 37960-79-5

Physical Properties

Property code	Value	Unit	Source
gf	-264.86	kJ/mol	Joback Method
hf	-414.98	kJ/mol	Joback Method
hfus	15.98	kJ/mol	Joback Method
hvap	64.05	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.778		Crippen Method
mcvol	129.580	ml/mol	McGowan Method
pc	4041.50	kPa	Joback Method
tb	599.82	K	Joback Method
tc	816.20	K	Joback Method
tf	338.52	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.06	J/mol×K	599.82	Joback Method
cpg	279.76	J/mol×K	635.88	Joback Method
cpg	286.87	J/mol×K	671.95	Joback Method
cpg	293.43	J/mol×K	708.01	Joback Method
cpg	299.47	J/mol×K	744.07	Joback Method
cpg	305.02	J/mol×K	780.13	Joback Method
cpg	310.12	J/mol×K	816.20	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=C37960795&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume