

2-Hydroxyethyl alpha,alpha-dichloro propionate

Inchi:	InChI=1S/C5H8Cl2O3/c1-5(6,7)4(9)10-3-2-8/h8H,2-3H2,1H3
InchiKey:	YGFNQSRXYGZCGF-UHFFFAOYSA-N
Formula:	C5H8Cl2O3
SMILES:	CC(Cl)(Cl)C(=O)OCCO
Mol. weight [g/mol]:	187.02
CAS:	90139-63-2

Physical Properties

Property code	Value	Unit	Source
gf	-400.54	kJ/mol	Joback Method
hf	-583.79	kJ/mol	Joback Method
hfus	16.56	kJ/mol	Joback Method
hvap	60.03	kJ/mol	Joback Method
log10ws	-0.95		Crippen Method
logp	0.716		Crippen Method
mcvol	119.100	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
tb	553.90	K	Joback Method
tc	746.77	K	Joback Method
tf	341.35	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.94	J/molxK	553.90	Joback Method
cpg	259.37	J/molxK	586.04	Joback Method
cpg	266.35	J/molxK	618.19	Joback Method
cpg	272.91	J/molxK	650.33	Joback Method
cpg	279.06	J/molxK	682.48	Joback Method
cpg	284.82	J/molxK	714.62	Joback Method
cpg	290.21	J/molxK	746.77	Joback Method
dvisc	0.0061695	Paxs	341.35	Joback Method
dvisc	0.0023839	Paxs	376.78	Joback Method

dvisc	0.0010847	Paxs	412.20	Joback Method
dvisc	0.0005590	Paxs	447.62	Joback Method
dvisc	0.0003175	Paxs	483.05	Joback Method
dvisc	0.0001949	Paxs	518.47	Joback Method
dvisc	0.0001273	Paxs	553.90	Joback Method

Sources

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=C90139632&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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