

Propanoic acid, 2,2-dichloro-, 1,2-ethanediyl ester

Other names:	Ethylene glycol bis(alpha,alpha-dichloropropionate)
Inchi:	InChI=1S/C8H10Cl4O4/c1-7(9,10)5(13)15-3-4-16-6(14)8(2,11)12/h3-4H2,1-2H3
InchiKey:	HDVMFCLSSJBSOM-UHFFFAOYSA-N
Formula:	C8H10Cl4O4
SMILES:	CC(Cl)(Cl)C(=O)OCCOC(=O)C(C)(Cl)Cl
Mol. weight [g/mol]:	311.98
CAS:	54934-49-5

Physical Properties

Property code	Value	Unit	Source
gf	-493.40	kJ/mol	Joback Method
hf	-778.51	kJ/mol	Joback Method
hfus	24.01	kJ/mol	Joback Method
hvap	66.66	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.460		Crippen Method
mcvol	187.420	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
tb	678.28	K	Joback Method
tc	900.11	K	Joback Method
tf	448.76	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.36	J/mol×K	678.28	Joback Method
cpg	433.76	J/mol×K	715.25	Joback Method
cpg	442.38	J/mol×K	752.22	Joback Method
cpg	450.26	J/mol×K	789.19	Joback Method
cpg	457.44	J/mol×K	826.17	Joback Method
cpg	463.97	J/mol×K	863.14	Joback Method
cpg	469.88	J/mol×K	900.11	Joback Method
dvisc	0.0011156	Pa×s	448.76	Joback Method

dvisc	0.0006638	Pa×s	487.01	Joback Method
dvisc	0.0004259	Pa×s	525.27	Joback Method
dvisc	0.0002903	Pa×s	563.52	Joback Method
dvisc	0.0002077	Pa×s	601.77	Joback Method
dvisc	0.0001547	Pa×s	640.03	Joback Method
dvisc	0.0001191	Pa×s	678.28	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=C54934495&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
mcvol:	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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