

Acetic acid, chloro-, 1-methyl-1,2-ethanediyl ester

Other names:	1,2-Bis(chloroacetoxy)propane Chloroacetic acid, 1,2-propanediol diester
Inchi:	InChI=1S/C7H10Cl2O4/c1-5(13-7(11)3-9)4-12-6(10)2-8/h5H,2-4H2,1H3
InchiKey:	RVKVLMMCZLSUGU-UHFFFAOYSA-N
Formula:	C7H10Cl2O4
SMILES:	CC(COC(=O)CCl)OC(=O)CCl
Mol. weight [g/mol]:	229.06
CAS:	42831-64-1

Physical Properties

Property code	Value	Unit	Source
gf	-486.08	kJ/mol	Joback Method
hf	-714.17	kJ/mol	Joback Method
hfus	24.33	kJ/mol	Joback Method
hvap	57.87	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.939		Crippen Method
mvol	148.850	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
tb	586.56	K	Joback Method
tc	785.49	K	Joback Method
tf	357.81	K	Joback Method
vc	0.568	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.69	J/mol×K	586.56	Joback Method
cpg	336.43	J/mol×K	619.72	Joback Method
cpg	345.69	J/mol×K	652.87	Joback Method
cpg	354.48	J/mol×K	686.03	Joback Method
cpg	362.79	J/mol×K	719.18	Joback Method
cpg	370.60	J/mol×K	752.34	Joback Method
cpg	377.92	J/mol×K	785.49	Joback Method

dvisc	0.0021007	Paxs	357.81	Joback Method
dvisc	0.0011981	Paxs	395.94	Joback Method
dvisc	0.0007542	Paxs	434.06	Joback Method
dvisc	0.0005116	Paxs	472.18	Joback Method
dvisc	0.0003677	Paxs	510.31	Joback Method
dvisc	0.0002767	Paxs	548.43	Joback Method
dvisc	0.0002161	Paxs	586.56	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=C42831641&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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