

1,3-Propanediol bis(alpha,alpha-di-chloropropionate)

Inchi:	InChI=1S/C9H12Cl4O4/c1-8(10,11)6(14)16-4-3-5-17-7(15)9(2,12)13/h3-5H2,1-2H3
InchiKey:	MFPNTKLWBHEOMV-UHFFFAOYSA-N
Formula:	C9H12Cl4O4
SMILES:	CC(Cl)(Cl)C(=O)OCCOC(=O)C(C)(Cl)Cl
Mol. weight [g/mol]:	326.00

Physical Properties

Property code	Value	Unit	Source
gf	-484.98	kJ/mol	Joback Method
hf	-799.15	kJ/mol	Joback Method
hfus	26.60	kJ/mol	Joback Method
hvap	68.89	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.850		Crippen Method
mcvol	201.510	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
tb	701.16	K	Joback Method
tc	919.31	K	Joback Method
tf	460.03	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.33	J/molxK	701.16	Joback Method
cpg	483.38	J/molxK	737.52	Joback Method
cpg	492.63	J/molxK	773.88	Joback Method
cpg	501.11	J/molxK	810.23	Joback Method
cpg	508.88	J/molxK	846.59	Joback Method
cpg	515.97	J/molxK	882.95	Joback Method
cpg	522.42	J/molxK	919.31	Joback Method
dvisc	0.0009971	Paxs	460.03	Joback Method
dvisc	0.0005843	Paxs	500.22	Joback Method
dvisc	0.0003707	Paxs	540.41	Joback Method

dvisc	0.0002504	Paxs	580.60	Joback Method
dvisc	0.0001780	Paxs	620.78	Joback Method
dvisc	0.0001319	Paxs	660.97	Joback Method
dvisc	0.0001012	Paxs	701.16	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=B6001970&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i

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
hvac:	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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