

Propane, 1,1'-oxybis[2-chloro-

Other names:	Bis(2-chloropropyl)ether Propane, 1,1'-oxybis*2-chloro- 2,2'-Dichloropropyl propyl ether
Inchi:	InChI=1S/C6H12Cl2O/c1-5(7)3-9-4-6(2)8/h5-6H,3-4H2,1-2H3
InchiKey:	LTJNJOSNHALAPB-UHFFFAOYSA-N
Formula:	C6H12Cl2O
SMILES:	CC(Cl)COCC(C)Cl
Mol. weight [g/mol]:	171.06
CAS:	54460-96-7

Physical Properties

Property code	Value	Unit	Source
gf	-134.10	kJ/mol	Joback Method
hf	-341.43	kJ/mol	Joback Method
hfus	13.83	kJ/mol	Joback Method
hvap	39.35	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	2.258		Crippen Method
mcvol	125.750	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
rinpol	1048.00		NIST Webbook
rinpol	1055.00		NIST Webbook
tb	433.08	K	Joback Method
tc	621.21	K	Joback Method
tf	209.45	K	Joback Method
vc	0.475	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.53	J/mol×K	433.08	Joback Method
cpg	245.04	J/mol×K	464.43	Joback Method
cpg	255.15	J/mol×K	495.79	Joback Method
cpg	264.85	J/mol×K	527.14	Joback Method

cpg	274.14	J/mol×K	558.50	Joback Method
cpg	283.05	J/mol×K	589.85	Joback Method
cpg	291.56	J/mol×K	621.21	Joback Method
dvisc	0.0084256	Paxs	209.45	Joback Method
dvisc	0.0030348	Paxs	246.72	Joback Method
dvisc	0.0014291	Paxs	283.99	Joback Method
dvisc	0.0008015	Paxs	321.26	Joback Method
dvisc	0.0005069	Paxs	358.54	Joback Method
dvisc	0.0003495	Paxs	395.81	Joback Method
dvisc	0.0002569	Paxs	433.08	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C54460967&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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