Bis(2-chloropropyl)ether

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]: 171.07

Physical Properties

Property code	Value	Unit	Source
af	0.4418		Cheméo Relay (1.0)
gf	-134.10	kJ/mol	Joback Method
hf	-371.67	kJ/mol	Cheméo Relay (1.0)
hfus	13.83	kJ/mol	Joback Method
hvap	50.51	kJ/mol	Cheméo Relay (1.0)
ie	9.97	eV	Cheméo Relay (1.0)
log10ws	-2.35		Cheméo Relay (1.0)
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	456.78	K	Cheméo Relay (1.0)
tc	647.23	K	Cheméo Relay (1.0)
tf	242.47	K	Cheméo Relay (1.0)
vc	0.446	m3/kmol	Cheméo Relay (1.0)

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	Pa×s	209.45	Joback Method
dvisc	0.0030348	Pa×s	246.72	Joback Method
dvisc	0.0014291	Pa×s	283.99	Joback Method
dvisc	0.0008015	Pa×s	321.26	Joback Method
dvisc	0.0005069	Pa×s	358.54	Joback Method
dvisc	0.0003495	Pa×s	395.81	Joback Method
dvisc	0.0002569	Pa×s	433.08	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54460967&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor

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

ie: Ionization energy

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