2,2-BIS(CHLOROMETHYL)-1-PROPANOL

Other names: 1-Propanol, 3-chloro-2-(chloromethyl)-2-methyl-
3-chloro-2-(chloromethyl)-2-methylpropan-1-ol
Inchi: InChI=1S/C5H10Cl2O/c1-5(2-6,3-7)4-8/h8H,2-4H2,1H3
InchiKey: DOANJBQUOFJQHC-UHFFFAOYSA-N
Formula: C5H10Cl2O
SMILES: CC(CO)(CCl)CCl
Mol. weight [g/mol]: 157.04

Physical Properties

Property code	Value	Unit	Source
af	0.5858		Cheméo Relay (1.0)
gf	-166.62	kJ/mol	Joback Method
hf	-360.21	kJ/mol	Cheméo Relay (1.0)
hfus	13.77	kJ/mol	Joback Method
hvap	67.76	kJ/mol	Cheméo Relay (1.0)
ie	10.01	eV	Cheméo Relay (1.0)
log10ws	-1.40		Cheméo Relay (1.0)
logp	1.463		Crippen Method
mcvol	111.660	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	486.37	K	Cheméo Relay (1.0)
tc	709.50	K	Cheméo Relay (1.0)
tf	345.03	K	Cheméo Relay (1.0)
vc	0.379	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.53	J/mol×K	477.61	Joback Method
cpg	264.51	J/mol×K	662.64	Joback Method
cpg	258.27	J/mol×K	631.80	Joback Method
cpg	251.63	J/mol×K	600.96	Joback Method
cpg	244.56	J/mol×K	570.13	Joback Method
cpg	237.03	J/mol×K	539.29	Joback Method

cpg	229.03	J/mol×K	508.45	Joback Method
dvisc	0.0013875	Pa×s	373.40	Joback Method
dvisc	0.0002289	Pa×s	477.61	Joback Method
dvisc	0.0003798	Pa×s	442.87	Joback Method
dvisc	0.0006870	Pa×s	408.14	Joback Method
dvisc	0.0339499	Pa×s	269.19	Joback Method
dvisc	0.0032371	Pa×s	338.66	Joback Method
dvisc	0.0091657	Pa×s	303.93	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.70	K	1.60	NIST Webbook

Sources

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):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5355544&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume