

# 2,2-Bis(chloromethyl)-1-propanol

<b>Other names:</b>	1-Propanol, 3-chloro-2-(chloromethyl)-2-methyl-3-chloro-2-(chloromethyl)-2-methylpropan-1-ol
<b>Inchi:</b>	InChI=1S/C5H10Cl2O/c1-5(2-6,3-7)4-8/h8H,2-4H2,1H3
<b>InchiKey:</b>	DOANJBQUOFJQHC-UHFFFAOYSA-N
<b>Formula:</b>	C5H10Cl2O
<b>SMILES:</b>	CC(CO)(CCI)CCI
<b>Mol. weight [g/mol]:</b>	157.04
<b>CAS:</b>	5355-54-4

## Physical Properties

Property code	Value	Unit	Source
gf	-166.62	kJ/mol	Joback Method
hf	-338.99	kJ/mol	Joback Method
hfus	13.77	kJ/mol	Joback Method
hvap	50.88	kJ/mol	Joback Method
log10ws	-1.24		Crippen Method
logp	1.463		Crippen Method
mvol	111.660	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	477.61	K	Joback Method
tc	662.64	K	Joback Method
tf	269.19	K	Joback Method
vc	0.421	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.53	J/molxK	477.61	Joback Method
cpg	258.27	J/molxK	631.80	Joback Method
cpg	251.63	J/molxK	600.96	Joback Method
cpg	244.56	J/molxK	570.13	Joback Method
cpg	237.03	J/molxK	539.29	Joback Method
cpg	229.03	J/molxK	508.45	Joback Method
cpg	264.51	J/molxK	662.64	Joback Method

dvisc	0.0002289	Paxs	477.61	Joback Method
dvisc	0.0003798	Paxs	442.87	Joback Method
dvisc	0.0006870	Paxs	408.14	Joback Method
dvisc	0.0013875	Paxs	373.40	Joback Method
dvisc	0.0032371	Paxs	338.66	Joback Method
dvisc	0.0091657	Paxs	303.93	Joback Method
dvisc	0.0339499	Paxs	269.19	Joback Method

## Pressure Dependent Properties

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

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5355544&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5355544&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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