

1-Propanol, 2,3-dichloro-

Other names:	1,2-Dichloro-3-propanol 1,2-Dichloropropanol-3 2,3-Dichloro-1-propanol 2,3-Dichloropropanol 2,3-dichloropropan-1-ol Glycerol «alpha»,«beta»-dichlorohydrin Glycerol Â«alphaÂ»,Â«betaÂ»-dichlorohydrin Glyceryl dichlorohydrin «alpha»,«beta»-Dichlorohydrin «beta»-Dichlorohydrin Â«alphaÂ»,Â«betaÂ»-Dichlorohydrin Â«betaÂ»-Dichlorohydrin
Inchi:	InChI=1S/C3H6Cl2O/c4-1-3(5)2-6/h3,6H,1-2H2
InchiKey:	ZXCYIJGIGSDJQQ-UHFFFAOYSA-N
Formula:	C3H6Cl2O
SMILES:	OCC(Cl)CCl
Mol. weight [g/mol]:	128.99
CAS:	616-23-9

Physical Properties

Property code	Value	Unit	Source
chl	-1704.00 ± 1.00	kJ/mol	NIST Webbook
chl	-1722.96	kJ/mol	NIST Webbook
gf	-188.74	kJ/mol	Joback Method
hf	-316.00 ± 4.60	kJ/mol	NIST Webbook
hfl	-381.00 ± 2.00	kJ/mol	NIST Webbook
hfus	12.49	kJ/mol	Joback Method
hvap	47.33	kJ/mol	Joback Method
log10ws	-0.76		Crippen Method
logp	0.825		Crippen Method
mcvol	83.480	ml/mol	McGowan Method
pc	4565.38	kPa	Joback Method
rinpol	959.00		NIST Webbook
rinpol	959.00		NIST Webbook
tb	456.00 ± 1.00	K	NIST Webbook
tc	615.83	K	Joback Method
tf	229.23	K	Joback Method

vc	0.315	m ³ /kmol	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.09	J/mol×K	585.63	Joback Method
cpg	171.37	J/mol×K	615.83	Joback Method
cpg	142.19	J/mol×K	434.64	Joback Method
cpg	147.67	J/mol×K	464.84	Joback Method
cpg	152.89	J/mol×K	495.04	Joback Method
cpg	157.86	J/mol×K	525.23	Joback Method
cpg	162.59	J/mol×K	555.43	Joback Method
dvisc	0.0003215	Pa×s	434.64	Joback Method
dvisc	0.0005461	Pa×s	400.40	Joback Method
dvisc	0.0828767	Pa×s	229.23	Joback Method
dvisc	0.0180080	Pa×s	263.47	Joback Method
dvisc	0.0055588	Pa×s	297.70	Joback Method
dvisc	0.0021867	Pa×s	331.94	Joback Method
dvisc	0.0010242	Pa×s	366.17	Joback Method
hvapt	65.30 ± 4.20	kJ/mol	293.00	NIST Webbook
hvapt	48.50	kJ/mol	401.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.75789e+01
Coeff. B	-5.91000e+03
Temperature range (K), min.	341.79
Temperature range (K), max.	481.77

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C616239&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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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