

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 «alpha», «beta»-dichlorohydrin Glyceryl dichlorohydrin «alpha», «beta»-Dichlorohydrin «beta»-Dichlorohydrin «alpha», «beta»-Dichlorohydrin «beta»-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

Temperature Dependent Properties

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C616239&Units=SI>

The Yaws Handbook of Vapor

Pressure:
Crippen Method:

Crippen Method:

Joback Method:

McGowan Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

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

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

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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