2-Propanol, 1,3-dichloro-

Other names:	.alpha.,.gamma.-dichlorohydrin
	.alpha.-dichlorohydrin
	1,3-Dichloro-2-hydroxypropane
	1,3-Dichloro-2-propanol
	1,3-Dichlorohydrin
	1,3-Dichloroisopropanol
	1,3-Dichloroisopropyl alcohol
	1,3-Dichloropropan-2-ol
	1,3-Dichloropropanol-2
	2-Chloro-1-(chloromethyl)ethanol
	Dichlorohydrin
	Enodrin
	Glycerol 1,3-dichlorohydrin
	Glycerol «alpha»,«gamma»-dichlorohydrin
	Glycerol Â«alphaÂ»,Â«gammaÂ»-dichlorohydrin
	NSC 70982
	Propylene dichlorohydrin
	S-Dichloroisopropyl alcohol
	S-Glycerol dichlorohydrin
	U 25,354
	UN 2750
	glycerol-.alpha.,.gamma.-dichlorohydrin
	glycerol-1,3-dichlorohydrin
	sym-Dichloroisopropyl alcohol
	sym-Glycerol dichlorohydrin
	«alpha»,«gamma»-Dichlorohydrin
	«alpha»-Dichlorohydrin
	Â«alphaÂ»,Â«gammaÂ»-Dichlorohydrin
	Â«alphaÂ»-Dichlorohydrin
Inchi:	InChI=1S/C3H6Cl2O/c4-1-3(6)2-5/h3,6H,1-2H2
InchiKey:	DEWLEGDTCGBNGU-UHFFFAOYSA-N
Formula:	C3H6Cl2O
SMILES:	OC(CCl)CCl
Mol. weight [g/mol]:	128.99
CAS:	96-23-1

Physical Properties

Property code	Value	Unit	Source
chl	-1700.00 ± 1.00	kJ/mol	NIST Webbook
chl	-1701.06 ± 0.12	kJ/mol	NIST Webbook
gf	-188.74	kJ/mol	Joback Method
hf	-294.24	kJ/mol	Joback Method
hfl	-385.00 ± 1.00	kJ/mol	NIST Webbook
hfus	12.49	kJ/mol	Joback Method
hvap	47.33	kJ/mol	Joback Method
log10ws	-0.11		Aqueous Solubility Prediction Method
logp	0.825		Crippen Method
mcvol	83.480	ml/mol	McGowan Method
pc	4565.38	kPa	Joback Method
rinpol	873.00		NIST Webbook
rinpol	852.90		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	863.00		NIST Webbook
ripol	1765.00		NIST Webbook
tb	448.30 ± 0.50	K	NIST Webbook
tb	447.00	K	NIST Webbook
tb	447.50	K	NIST Webbook
tb	448.30 ± 0.50	K	NIST Webbook
tb	448.30 ± 0.50	K	NIST Webbook
tc	615.83	K	Joback Method
tf	229.23	K	Joback Method
vc	0.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	167.09	J/mol×K	585.63	Joback Method
cpg	171.37	J/mol×K	615.83	Joback Method

dvisc	0.0005461	Pa×s	400.40	Joback Method
dvisc	0.0010242	Pa×s	366.17	Joback Method
dvisc	0.0021867	Pa×s	331.94	Joback Method
dvisc	0.0055588	Pa×s	297.70	Joback Method
dvisc	0.0180080	Pa×s	263.47	Joback Method
dvisc	0.0003215	Pa×s	434.64	Joback Method
dvisc	0.0828767	Pa×s	229.23	Joback Method
hvapt	50.40	kJ/mol	374.50	NIST Webbook
rhol	1356.74	kg/m3	298.15	The study of excess molar volumes and related properties for binary mixtures containing benzyl alcohol and 1,3-dichloro-2-propanol with vinyl acetate, ethyl acetate and t-butyl acetate at T = 293.15 to 313.15 K and P = 0.087 MPa
rhol	1350.72	kg/m3	303.15	The study of excess molar volumes and related properties for binary mixtures containing benzyl alcohol and 1,3-dichloro-2-propanol with vinyl acetate, ethyl acetate and t-butyl acetate at T = 293.15 to 313.15 K and P = 0.087 MPa
rhol	1344.71	kg/m3	308.15	The study of excess molar volumes and related properties for binary mixtures containing benzyl alcohol and 1,3-dichloro-2-propanol with vinyl acetate, ethyl acetate and t-butyl acetate at T = 293.15 to 313.15 K and P = 0.087 MPa

rhol	1362.66	kg/m3	293.15	The study of excess molar volumes and related properties for binary mixtures containing benzyl alcohol and 1,3-dichloro-2-propanol with vinyl acetate, ethyl acetate and t-butyl acetate at T = 293.15 to 313.15 K and P = 0.087 MPa
rhol	1338.56	kg/m3	313.15	Volumetric properties for binary and ternary mixtures of allyl alcohol, 1,3-dichloro-2-propanol and 1-ethyl-3-methyl imidazolium ethyl sulfate [Emim][EtSO4] from T = 298.15 to 318.15 K at ambient pressure
rhol	1344.61	kg/m3	308.15	Volumetric properties for binary and ternary mixtures of allyl alcohol, 1,3-dichloro-2-propanol and 1-ethyl-3-methyl imidazolium ethyl sulfate [Emim][EtSO4] from T = 298.15 to 318.15 K at ambient pressure
rhol	1350.55	kg/m3	303.15	Volumetric properties for binary and ternary mixtures of allyl alcohol, 1,3-dichloro-2-propanol and 1-ethyl-3-methyl imidazolium ethyl sulfate [Emim][EtSO4] from T = 298.15 to 318.15 K at ambient pressure

rhol	1356.46	kg/m3	298.15	Volumetric properties for binary and ternary mixtures of allyl alcohol, 1,3-dichloro-2-propanol and 1-ethyl-3-methyl imidazolium ethyl sulfate [Emim][EtSO4] from T = 298.15 to 318.15 K at ambient pressure
rhol	1338.65	kg/m3	313.15	The study of excess molar volumes and related properties for binary mixtures containing benzyl alcohol and 1,3-dichloro-2-propanol with vinyl acetate, ethyl acetate and t-butyl acetate at T = 293.15 to 313.15 K and P = 0.087 MPa
rhol	1332.47	kg/m3	318.15	Volumetric properties for binary and ternary mixtures of allyl alcohol, 1,3-dichloro-2-propanol and 1-ethyl-3-methyl imidazolium ethyl sulfate [Emim][EtSO4] from T = 298.15 to 318.15 K at ambient pressure

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.72693e+01
Coeff. B	-5.45806e+03
Coeff. C	-1.60670e+01
Temperature range (K), min.	337.47
Temperature range (K), max.	472.51

Sources

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
Liquid Liquid Equilibria for the System Water + 1,3-Dichloro-2-propanol + Epichlorohydrin from (283.2 to 303.2) K:	https://www.doi.org/10.1021/je400681a
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96231&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Volumetric properties for binary and ternary mixtures of allyl alcohol, 1,3-dichloro-2-propanol and 1-ethyl-3-methyl imidazolium ethyl sulfate [emim][EtSO4] from T = 298.15 to 318.15 K at ambient pressure:	https://www.doi.org/10.1016/j.tca.2015.04.027
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The study of excess molar volumes and related properties for binary mixtures containing benzyl alcohol and 1,3-dichloro-2-propanol with vinyl acetate, ethyl acetate and t-butyl acetate at T = 293.15 to 313.15 K and P = 0.083 MPa:	https://www.doi.org/10.1016/j.tca.2016.04.001

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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/29-224-1/2-Propanol-1-3-dichloro.pdf

Generated by Cheméo on 2024-04-20 09:19:16.72612668 +0000 UTC m=+15894005.646703996.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.