

2,2-Propanediol, 1,3-dichloro-

Inchi:	InChI=1S/C3H6Cl2O2/c4-1-3(6,7)2-5/h6-7H,1-2H2
InchiKey:	BJCFYPFSEIJWLQ-UHFFFAOYSA-N
Formula:	C3H6Cl2O2
SMILES:	OC(O)(CCl)CCl
Mol. weight [g/mol]:	144.99
CAS:	82598-72-9

Physical Properties

Property code	Value	Unit	Source
gf	-320.28	kJ/mol	Joback Method
hf	-449.94	kJ/mol	Joback Method
hfus	12.68	kJ/mol	Joback Method
hvap	63.10	kJ/mol	Joback Method
log10ws	-0.52		Crippen Method
logp	0.145		Crippen Method
mcvol	89.350	ml/mol	McGowan Method
pc	5273.90	kPa	Joback Method
tb	524.03	K	Joback Method
tc	703.82	K	Joback Method
tf	307.47	K	Joback Method
vc	0.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.00	J/molxK	524.03	Joback Method
cpg	183.04	J/molxK	553.99	Joback Method
cpg	187.73	J/molxK	583.96	Joback Method
cpg	192.10	J/molxK	613.92	Joback Method
cpg	196.18	J/molxK	643.89	Joback Method
cpg	199.98	J/molxK	673.85	Joback Method
cpg	203.52	J/molxK	703.82	Joback Method
dvisc	0.0474602	Paxs	307.47	Joback Method
dvisc	0.0098056	Paxs	343.56	Joback Method

dvisc	0.0027342	Paxs	379.66	Joback Method
dvisc	0.0009517	Paxs	415.75	Joback Method
dvisc	0.0003921	Paxs	451.84	Joback Method
dvisc	0.0001842	Paxs	487.94	Joback Method
dvisc	0.0000960	Paxs	524.03	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82598729&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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