Ethanol, 2,2-dichloro-

Other names:	2,2-dichloroethanol
	Dichloroethanol
Inchi:	InChI=1S/C2H4Cl2O/c3-2(4)1-5/h2,5H,1H2
InchiKey:	IDJOCJAIQSKSOP-UHFFFAOYSA-N
Formula:	C2H4Cl2O
SMILES:	OCC(Cl)Cl
Mol. weight [g/mol]:	114.96
CAS:	598-38-9

Physical Properties

Property code	Value	Unit	Source
gf	-197.16	kJ/mol	Joback Method
hf	-273.60	kJ/mol	Joback Method
hfus	9.89	kJ/mol	Joback Method
hvap	45.11	kJ/mol	Joback Method
log10ws	-0.84		Crippen Method
logp	0.782		Crippen Method
mcvol	69.390	ml/mol	McGowan Method
pc	5220.69	kPa	Joback Method
rinpol	742.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	672.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	690.00		NIST Webbook
ripol	1616.00		NIST Webbook
ripol	1623.00		NIST Webbook
ripol	1604.00		NIST Webbook
ripol	1633.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1601.00		NIST Webbook
ripol	1609.00		NIST Webbook
tb	419.20	K	NIST Webbook

tc	594.31	K	Joback Method
tf	217.96	K	Joback Method
vc	0.259	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	108.05	J/mol×K	411.76	Joback Method
cpg	126.38	J/mol×K	563.89	Joback Method
cpg	123.08	J/mol×K	533.46	Joback Method
cpg	119.61	J/mol×K	503.04	Joback Method
cpg	115.95	J/mol×K	472.61	Joback Method
cpg	112.10	J/mol×K	442.19	Joback Method
cpg	129.51	J/mol×K	594.31	Joback Method
dvisc	0.0003925	Pa×s	411.76	Joback Method
dvisc	0.0006717	Pa×s	379.46	Joback Method
dvisc	0.0012703	Pa×s	347.16	Joback Method
dvisc	0.0027379	Pa×s	314.86	Joback Method
dvisc	0.0070336	Pa×s	282.56	Joback Method
dvisc	0.0230524	Pa×s	250.26	Joback Method
dvisc	0.1074113	Pa×s	217.96	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=C598389&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Henry s Law Constants of Organic Compounds in Water and n-Octane at T = 293.2 K:	https://www.doi.org/10.1021/je900711h

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
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