

# 2,2-Dichloroethanol, acetate

<b>Other names:</b>	Ethanol, 2,2-dichloro-, 1-acetate Acetic acid 2,2-dichloroethyl ester Ethanol, 2,2-dichloro-, acetate 2,2-Dichloroethyl acetate
<b>Inchi:</b>	InChI=1S/C4H6Cl2O2/c1-3(7)8-2-4(5)6/h4H,2H2,1H3
<b>InchiKey:</b>	DBEYJHSHTGBZIM-UHFFFAOYSA-N
<b>Formula:</b>	C4H6Cl2O2
<b>SMILES:</b>	CC(=O)OCC(Cl)Cl
<b>Mol. weight [g/mol]:</b>	157.00
<b>CAS:</b>	53942-53-3

## Physical Properties

Property code	Value	Unit	Source
gf	-277.42	kJ/mol	Joback Method
hf	-407.45	kJ/mol	Joback Method
hfus	13.77	kJ/mol	Joback Method
hvap	42.04	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	1.353		Crippen Method
mcvol	99.140	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
rinpol	924.80		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	899.00		NIST Webbook
ripol	1447.00		NIST Webbook
ripol	1447.00		NIST Webbook
ripol	1426.00		NIST Webbook
ripol	1480.00		NIST Webbook
ripol	1451.00		NIST Webbook
ripol	1465.00		NIST Webbook
tb	441.63	K	Joback Method
tc	640.84	K	Joback Method
tf	251.84	K	Joback Method
vc	0.376	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.11	J/molxK	441.63	Joback Method
cpg	178.98	J/molxK	474.83	Joback Method
cpg	185.57	J/molxK	508.03	Joback Method
cpg	191.90	J/molxK	541.23	Joback Method
cpg	197.95	J/molxK	574.44	Joback Method
cpg	203.72	J/molxK	607.64	Joback Method
cpg	209.22	J/molxK	640.84	Joback Method
dvisc	0.0039286	Paxs	251.84	Joback Method
dvisc	0.0020794	Paxs	283.47	Joback Method
dvisc	0.0012506	Paxs	315.10	Joback Method
dvisc	0.0008253	Paxs	346.74	Joback Method
dvisc	0.0005838	Paxs	378.37	Joback Method
dvisc	0.0004356	Paxs	410.00	Joback Method
dvisc	0.0003390	Paxs	441.63	Joback Method

## Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C53942533&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C53942533&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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