

# 1-Propanol, 2,2-dimethyl-, acetate

<b>Other names:</b>	2,2-Dimethyl-1-propanol acetate 2,2-Dimethylpropyl acetate 2,2-Dimethylpropyl ethanoate Acetic acid, neopentyl ester Neopentyl acetate Neopentyl alcohol, acetate
<b>Inchi:</b>	InChI=1S/C7H14O2/c1-6(8)9-5-7(2,3)4/h5H2,1-4H3
<b>InchiKey:</b>	QLNYTCSELYEEPV-UHFFFAOYSA-N
<b>Formula:</b>	C7H14O2
<b>SMILES:</b>	CC(=O)OCC(C)(C)C
<b>Mol. weight [g/mol]:</b>	130.18
<b>CAS:</b>	926-41-0

## Physical Properties

Property code	Value	Unit	Source
gf	-223.02	kJ/mol	Joback Method
hf	-441.36	kJ/mol	Joback Method
hfus	9.26	kJ/mol	Joback Method
hvap	39.04	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.596		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	816.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	810.90		NIST Webbook
tb	432.62	K	Joback Method
tc	620.42	K	Joback Method
tf	243.23	K	Joback Method
vc	0.441	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	306.89	J/molxK	620.42	Joback Method
cpg	241.05	J/molxK	432.62	Joback Method
cpg	253.38	J/molxK	463.92	Joback Method
cpg	265.15	J/molxK	495.22	Joback Method
cpg	276.37	J/molxK	526.52	Joback Method
cpg	287.06	J/molxK	557.82	Joback Method
cpg	297.22	J/molxK	589.12	Joback Method
dvisc	0.0002778	Paxs	432.62	Joback Method
dvisc	0.0047587	Paxs	243.23	Joback Method
dvisc	0.0022582	Paxs	274.80	Joback Method
dvisc	0.0012495	Paxs	306.36	Joback Method
dvisc	0.0007722	Paxs	337.93	Joback Method
dvisc	0.0005181	Paxs	369.49	Joback Method
dvisc	0.0003702	Paxs	401.06	Joback Method
hvapt	49.10	kJ/mol	350.50	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40131e+01
Coeff. B	-3.39501e+03
Coeff. C	-5.26700e+01
Temperature range (K), min.	300.02
Temperature range (K), max.	442.83

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<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=C926410&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C926410&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rinpol:</b>	Non-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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