

# Acetic acid, trans-4-methylcyclohexyl ester

<b>Inchi:</b>	InChI=1S/C9H16O2/c1-7-3-5-9(6-4-7)11-8(2)10/h7,9H,3-6H2,1-2H3
<b>InchiKey:</b>	VJBFCCCTSQEGMH-UHFFFAOYSA-N
<b>Formula:</b>	C9H16O2
<b>SMILES:</b>	CC(=O)OC1CCC(C)CC1
<b>Mol. weight [g/mol]:</b>	156.22

## Physical Properties

Property code	Value	Unit	Source
gf	-192.28	kJ/mol	Joback Method
hf	-439.91	kJ/mol	Joback Method
hfus	14.76	kJ/mol	Joback Method
hvap	44.90	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.128		Crippen Method
mvol	134.250	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
rinpol	1100.00		NIST Webbook
rinpol	1100.00		NIST Webbook
tb	496.49	K	Joback Method
tc	704.73	K	Joback Method
tf	266.49	K	Joback Method
vc	0.495	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.98	J/molxK	496.49	Joback Method
cpg	326.41	J/molxK	531.20	Joback Method
cpg	343.02	J/molxK	565.90	Joback Method
cpg	358.81	J/molxK	600.61	Joback Method
cpg	373.79	J/molxK	635.31	Joback Method
cpg	387.96	J/molxK	670.02	Joback Method
cpg	401.32	J/molxK	704.73	Joback Method
dvisc	0.0031798	Paxs	266.49	Joback Method

dvisc	0.0016403	Paxs	304.82	Joback Method
dvisc	0.0009810	Paxs	343.16	Joback Method
dvisc	0.0006505	Paxs	381.49	Joback Method
dvisc	0.0004650	Paxs	419.82	Joback Method
dvisc	0.0003516	Paxs	458.16	Joback Method
dvisc	0.0002776	Paxs	496.49	Joback Method

## 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=U368246&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368246&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>

## 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>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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