

# Propanoic acid, 2,2-dimethyl-, cyclohexyl ester

<b>Other names:</b>	2,2-Dimethylpropionic acid, cyclohexyl ester Cyclohexyl pivalate
<b>Inchi:</b>	InChI=1S/C11H20O2/c1-11(2,3)10(12)13-9-7-5-4-6-8-9/h9H,4-8H2,1-3H3
<b>InchiKey:</b>	WDCXGSMKFYMFCM-UHFFFAOYSA-N
<b>Formula:</b>	C11H20O2
<b>SMILES:</b>	CC(C)(C)C(=O)OC1CCCCC1
<b>Mol. weight [g/mol]:</b>	184.28
<b>CAS:</b>	29878-49-7

## Physical Properties

Property code	Value	Unit	Source
gf	-164.89	kJ/mol	Joback Method
hf	-469.60	kJ/mol	Joback Method
hfus	11.45	kJ/mol	Joback Method
h vap	59.00	kJ/mol	NIST Webbook
log10ws	-3.05		Crippen Method
logp	2.908		Crippen Method
m cvol	162.430	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
tb	543.69	K	Joback Method
tc	758.67	K	Joback Method
tf	295.69	K	Joback Method
vc	0.598	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.96	J/molxK	543.69	Joback Method
cpg	426.73	J/molxK	579.52	Joback Method
cpg	445.33	J/molxK	615.35	Joback Method
cpg	462.79	J/molxK	651.18	Joback Method
cpg	479.14	J/molxK	687.01	Joback Method
cpg	494.43	J/molxK	722.84	Joback Method
cpg	508.69	J/molxK	758.67	Joback Method

dvisc	0.0050998	Paxs	295.69	Joback Method
dvisc	0.0021528	Paxs	337.02	Joback Method
dvisc	0.0010972	Paxs	378.36	Joback Method
dvisc	0.0006386	Paxs	419.69	Joback Method
dvisc	0.0004096	Paxs	461.02	Joback Method
dvisc	0.0002826	Paxs	502.36	Joback Method
dvisc	0.0002063	Paxs	543.69	Joback Method

## Sources

<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=C29878497&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C29878497&amp;Units=SI</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>
<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>

## 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>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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