

# 3,3-dimethylcyclohex-6-en-1-yl propionate

<b>Inchi:</b>	InChI=1S/C11H18O2/c1-4-10(12)13-9-6-5-7-11(2,3)8-9/h6H,4-5,7-8H2,1-3H3
<b>InchiKey:</b>	AAJGKOFWDAXFFY-UHFFFAOYSA-N
<b>Formula:</b>	C11H18O2
<b>SMILES:</b>	CCC(=O)OC1=CCCC(C)(C)C1
<b>Mol. weight [g/mol]:</b>	182.26

## Physical Properties

Property code	Value	Unit	Source
gf	-152.89	kJ/mol	Joback Method
hf	-399.30	kJ/mol	Joback Method
hfus	13.40	kJ/mol	Joback Method
hvap	49.47	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.034		Crippen Method
mcvol	158.130	ml/mol	McGowan Method
pc	2611.07	kPa	Joback Method
rinpol	1360.00		NIST Webbook
tb	551.30	K	Joback Method
tc	764.81	K	Joback Method
tf	330.45	K	Joback Method
vc	0.593	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.71	J/molxK	551.30	Joback Method
cpg	401.63	J/molxK	586.89	Joback Method
cpg	417.59	J/molxK	622.47	Joback Method
cpg	432.70	J/molxK	658.06	Joback Method
cpg	447.04	J/molxK	693.64	Joback Method
cpg	460.71	J/molxK	729.23	Joback Method
cpg	473.80	J/molxK	764.81	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=R216345&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R216345&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>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>hvac:</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>mccol:</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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