

# Methyl-1,5,5-Trimethylbicyclo[4.1.0]heptan-7-carb

<b>Inchi:</b>	InChI=1S/C13H22O2/c1-12(2)6-5-7-13(3)8-9(10(12)13)11(14)15-4/h9-10H,5-8H2,1-4H3
<b>InchiKey:</b>	VJHJXUZMZATUAR-UHFFFAOYSA-N
<b>Formula:</b>	C13H22O2
<b>SMILES:</b>	COC(=O)C1CC2(C)CCCC(C)(C)C12
<b>Mol. weight [g/mol]:</b>	210.31

## Physical Properties

Property code	Value	Unit	Source
gf	-104.44	kJ/mol	Joback Method
hf	-433.37	kJ/mol	Joback Method
hfus	13.83	kJ/mol	Joback Method
hvap	50.94	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	3.012		Crippen Method
mcvol	179.750	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinsol	1258.00		NIST Webbook
tb	586.29	K	Joback Method
tc	805.67	K	Joback Method
tf	376.59	K	Joback Method
vc	0.679	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.76	J/molxK	586.29	Joback Method
cpg	509.83	J/molxK	622.85	Joback Method
cpg	528.72	J/molxK	659.42	Joback Method
cpg	546.65	J/molxK	695.98	Joback Method
cpg	563.86	J/molxK	732.54	Joback Method
cpg	580.56	J/molxK	769.11	Joback Method
cpg	596.98	J/molxK	805.67	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R229297&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R229297&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>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>mccvol:</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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