

# Tricyclo[3.3.1.1(3,7)]decane-2-ol-1-carboxylic acid, methyl ester

Inchi:	InChI=1S/C12H18O3/c1-15-11(14)12-5-7-2-8(6-12)4-9(3-7)10(12)13/h7-10,13H,2-6H2,1
InchiKey:	SEVMKXVZUKPSMQ-UHFFFAOYSA-N
Formula:	C12H18O3
SMILES:	COC(=O)C12CC3CC(CC(C3)C1O)C2
Mol. weight [g/mol]:	210.27
CAS:	41171-74-8

## Physical Properties

Property code	Value	Unit	Source
gf	-171.34	kJ/mol	Joback Method
hf	-501.24	kJ/mol	Joback Method
hfus	21.86	kJ/mol	Joback Method
hvap	66.28	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.347		Crippen Method
mcvol	160.670	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
tb	657.82	K	Joback Method
tc	864.56	K	Joback Method
tf	423.70	K	Joback Method
vc	0.610	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.22	J/molxK	657.82	Joback Method
cpg	504.99	J/molxK	692.28	Joback Method
cpg	519.94	J/molxK	726.73	Joback Method
cpg	534.20	J/molxK	761.19	Joback Method
cpg	547.94	J/molxK	795.65	Joback Method
cpg	561.28	J/molxK	830.10	Joback Method
cpg	574.38	J/molxK	864.56	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C41171748&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C41171748&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>
<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>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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