

# Tricyclo[3.2.1.1<sup>3,6</sup>]nonan-7-one

<b>Other names:</b>	Tricyclo[3.2.1.1
<b>Inchi:</b>	InChI=1S/C9H12O/c10-9-7-2-5-1-6(4-7)8(9)3-5/h5-8H,1-4H2
<b>InchiKey:</b>	QUXWGFTVVNVNFO-UHFFFAOYSA-N
<b>Formula:</b>	C9H12O
<b>SMILES:</b>	O=C1C2CC3CC(C2)C1C3
<b>Mol. weight [g/mol]:</b>	136.19
<b>CAS:</b>	17931-67-8

## Physical Properties

Property code	Value	Unit	Source
gf	76.85	kJ/mol	Joback Method
hf	-168.73	kJ/mol	Joback Method
hfus	14.05	kJ/mol	Joback Method
hvap	39.30	kJ/mol	Joback Method
ie	8.81	eV	NIST Webbook
log10ws	-1.59		Crippen Method
logp	1.621		Crippen Method
mcvol	106.660	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
tb	488.69	K	Joback Method
tc	715.13	K	Joback Method
tf	308.99	K	Joback Method
vc	0.416	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.05	J/molxK	488.69	Joback Method
cpg	281.88	J/molxK	526.43	Joback Method
cpg	298.49	J/molxK	564.17	Joback Method
cpg	313.97	J/molxK	601.91	Joback Method
cpg	328.39	J/molxK	639.65	Joback Method
cpg	341.83	J/molxK	677.39	Joback Method
cpg	354.38	J/molxK	715.13	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=C17931678&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17931678&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<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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