

# Bicyclo[2.2.2]oct-5-ene-2-carbonitrile, (1 «alpha»,2 «beta»,4 «alpha»)-

Inchi:	InChI=1S/C9H11N/c10-6-9-5-7-1-3-8(9)4-2-7/h1,3,7-9H,2,4-5H2/t7?,8?,9-/m0/s1
InchiKey:	WFLYMJQGKVLTO-HACHORDNSA-N
Formula:	C9H11N
SMILES:	N#CC1CC2C=CC1CC2
Mol. weight [g/mol]:	133.19
CAS:	3008-13-7

## Physical Properties

Property code	Value	Unit	Source
gf	277.63	kJ/mol	Joback Method
hf	153.00 ± 4.20	kJ/mol	NIST Webbook
hfus	14.93	kJ/mol	Joback Method
hvap	46.26	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.112		Crippen Method
mcvol	113.030	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
tb	523.91	K	Joback Method
tc	754.50	K	Joback Method
tf	281.54	K	Joback Method
vc	0.449	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.65	J/molxK	523.91	Joback Method
cpg	283.97	J/molxK	562.34	Joback Method
cpg	298.21	J/molxK	600.77	Joback Method
cpg	311.42	J/molxK	639.21	Joback Method
cpg	323.68	J/molxK	677.64	Joback Method
cpg	335.06	J/molxK	716.07	Joback Method
cpg	345.62	J/molxK	754.50	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3008137&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3008137&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>

# 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>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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