

# Bicyclo[2.2.2]oct-5-ene-2-carbonitrile, 3-methyl-, (1«alpha»,2«beta»,3«beta»,4«alpha»)- (exo,exo)

InChI: InChI=1S/C10H13N/c1-7-8-2-4-9(5-3,6)10(7)5-11/h7-10H,2-5H2,1H3/t7-,8?,9?,10-/m0/s  
InChIKey: ZFLTZPJOKVUDPQ-NFTFJBJSSA-N

Formula: C10H13N

SMILES: CC1C2CCC(CC2)C1C#N

Mol. weight [g/mol]: 147.22

CAS: 114718-71-7

## Physical Properties

Property code	Value	Unit	Source
gf	248.38	kJ/mol	Joback Method
hf	134.00	kJ/mol	NIST Webbook
hfus	17.37	kJ/mol	Joback Method
hvap	47.88	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.582		Crippen Method
mcvol	131.420	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
tb	542.96	K	Joback Method
tc	766.99	K	Joback Method
tf	287.81	K	Joback Method
vc	0.517	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.51	J/molxK	542.96	Joback Method
cpg	352.31	J/molxK	580.30	Joback Method
cpg	368.98	J/molxK	617.64	Joback Method
cpg	384.58	J/molxK	654.98	Joback Method
cpg	399.16	J/molxK	692.32	Joback Method
cpg	412.78	J/molxK	729.66	Joback Method
cpg	425.50	J/molxK	766.99	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=C114718717&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C114718717&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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