

# Propanedinitrile, 2-dicyclopropylmethylene-

<b>Inchi:</b>	InChI=1S/C10H10N2/c11-5-9(6-12)10(7-1-2-7)8-3-4-8/h7-8H,1-4H2
<b>InchiKey:</b>	WNHGKHKCOVLPMTU-UHFFFAOYSA-N
<b>Formula:</b>	C10H10N2
<b>SMILES:</b>	N#CC(C#N)=C(C1CC1)C1CC1
<b>Mol. weight [g/mol]:</b>	158.20
<b>CAS:</b>	13017-60-2

## Physical Properties

Property code	Value	Unit	Source
gf	484.30	kJ/mol	Joback Method
hf	323.27	kJ/mol	Joback Method
hfus	18.52	kJ/mol	Joback Method
hvap	58.75	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.150		Crippen Method
mcvol	128.500	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
tb	649.76	K	Joback Method
tc	890.71	K	Joback Method
tf	335.32	K	Joback Method
vc	0.543	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.61	J/mol×K	649.76	Joback Method
cpg	347.14	J/mol×K	689.92	Joback Method
cpg	357.78	J/mol×K	730.08	Joback Method
cpg	367.68	J/mol×K	770.23	Joback Method
cpg	376.96	J/mol×K	810.39	Joback Method
cpg	385.76	J/mol×K	850.55	Joback Method
cpg	394.22	J/mol×K	890.71	Joback Method

# Sources

<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=C13017602&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13017602&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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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