

# 3-(Cyclopropylamino)propionitrile

<b>Inchi:</b>	InChI=1S/C6H10N2/c7-4-1-5-8-6-2-3-6/h6,8H,1-3,5H2
<b>InchiKey:</b>	OZHWHTICSNFGBZ-UHFFFAOYSA-N
<b>Formula:</b>	C6H10N2
<b>SMILES:</b>	N#CCCNC1CC1
<b>Mol. weight [g/mol]:</b>	110.16
<b>CAS:</b>	58196-47-7

## Physical Properties

Property code	Value	Unit	Source
gf	282.96	kJ/mol	Joback Method
hf	123.98	kJ/mol	Joback Method
hfus	16.04	kJ/mol	Joback Method
hvap	45.78	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	0.652		Crippen Method
mvol	95.900	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
tb	495.67	K	Joback Method
tc	702.43	K	Joback Method
tf	292.97	K	Joback Method
vc	0.390	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.81	J/mol×K	495.67	Joback Method
cpg	225.51	J/mol×K	530.13	Joback Method
cpg	235.55	J/mol×K	564.59	Joback Method
cpg	244.97	J/mol×K	599.05	Joback Method
cpg	253.79	J/mol×K	633.51	Joback Method
cpg	262.08	J/mol×K	667.97	Joback Method
cpg	269.86	J/mol×K	702.43	Joback Method

# Sources

<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>
<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=C58196477&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C58196477&amp;Units=SI</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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