

# 1-Cyclohexene-1-acetonitrile

<b>Other names:</b>	Cyclohexenylacetonitrile 1-Cyclohexen-1-ylacetonitrile 1-Cyclohexenylacetonitrile cyclohex-1-ene-1-acetonitrile
<b>Inchi:</b>	InChI=1S/C8H11N/c9-7-6-8-4-2-1-3-5-8/h4H,1-3,5-6H2
<b>InchiKey:</b>	OYEXEQFKIPJKJK-UHFFFAOYSA-N
<b>Formula:</b>	C8H11N
<b>SMILES:</b>	N#CCC1=CCCCC1
<b>Mol. weight [g/mol]:</b>	121.18
<b>CAS:</b>	6975-71-9

## Physical Properties

Property code	Value	Unit	Source
gf	202.15	kJ/mol	Joback Method
hf	77.40	kJ/mol	Joback Method
hfus	9.58	kJ/mol	Joback Method
hvap	45.57	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.400		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
tb	512.88	K	Joback Method
tc	739.82	K	Joback Method
tf	269.81	K	Joback Method
vc	0.429	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.25	J/molxK	512.88	Joback Method
cpg	249.39	J/molxK	550.70	Joback Method
cpg	261.73	J/molxK	588.53	Joback Method
cpg	273.29	J/molxK	626.35	Joback Method
cpg	284.11	J/molxK	664.17	Joback Method

cpg	294.22	J/mol×K	701.99	Joback Method
cpg	303.66	J/mol×K	739.82	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	417.20	K	12.00	NIST Webbook
tbrp	384.00 ± 1.00	K	3.30	NIST Webbook

## 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=C6975719&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6975719&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>

## 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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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