

# Heptane nitrile

<b>Inchi:</b>	InChI=1S/C7H13N/c1-2-3-4-5-6-7-8/h2-6H2,1H3
<b>InchiKey:</b>	SDAXRHHPNYTELL-UHFFFAOYSA-N
<b>Formula:</b>	C7H13N
<b>SMILES:</b>	CCCCCCC#N
<b>Mol. weight [g/mol]:</b>	111.18

## Physical Properties

Property code	Value	Unit	Source
gf	141.24	kJ/mol	Joback Method
hf	-22.93	kJ/mol	Joback Method
hfus	15.39	kJ/mol	Joback Method
hvap	41.65	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.480		Crippen Method
mcvol	110.870	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
tb	461.64	K	Joback Method
tc	648.70	K	Joback Method
tf	233.64	K	Joback Method
vc	0.454	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.18	J/mol×K	461.64	Joback Method
cpg	239.70	J/mol×K	492.82	Joback Method
cpg	249.78	J/mol×K	523.99	Joback Method
cpg	259.42	J/mol×K	555.17	Joback Method
cpg	268.64	J/mol×K	586.35	Joback Method
cpg	277.45	J/mol×K	617.53	Joback Method
cpg	285.87	J/mol×K	648.70	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=B6000118&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6000118&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>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

Latest version available from:

<https://www.chemeo.com/cid/33-393-9/Heptane-nitrile.pdf>

Generated by Cheméo on 2024-04-26 03:30:06.545337751 +0000 UTC m=+16391455.465915068.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.