

# 4-Cyano-1-butyne

<b>Inchi:</b>	InChI=1S/C5H5N/c1-2-3-4-5-6/h1H,3-4H2
<b>InchiKey:</b>	VMUWIDHKAIGONP-UHFFFAOYSA-N
<b>Formula:</b>	C5H5N
<b>SMILES:</b>	C#CCCC#N
<b>Mol. weight [g/mol]:</b>	79.10
<b>CAS:</b>	19596-07-7

## Physical Properties

Property code	Value	Unit	Source
gf	347.47	kJ/mol	Joback Method
hf	310.25	kJ/mol	Joback Method
hfus	13.19	kJ/mol	Joback Method
hvap	37.06	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	0.923		Crippen Method
mcvol	74.090	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
tb	406.00	K	Joback Method
tc	611.08	K	Joback Method
tf	258.07	K	Joback Method
vc	0.303	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	127.83	J/molxK	406.00	Joback Method
cpg	133.70	J/molxK	440.18	Joback Method
cpg	139.26	J/molxK	474.36	Joback Method
cpg	144.53	J/molxK	508.54	Joback Method
cpg	149.51	J/molxK	542.72	Joback Method
cpg	154.22	J/molxK	576.90	Joback Method
cpg	158.68	J/molxK	611.08	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	333.00	K	1.30	NIST Webbook

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C19596077&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19596077&amp;Units=SI</a>
Crippen Method:	<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>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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