

# 3-(Butylamino)propionitrile

<b>Other names:</b>	3-Butylamino-propanenitrile
<b>Inchi:</b>	InChI=1S/C7H14N2/c1-2-3-6-9-7-4-5-8/h9H,2-4,6-7H2,1H3
<b>InchiKey:</b>	FPGVMJDQNJEAJM-UHFFFAOYSA-N
<b>Formula:</b>	C7H14N2
<b>SMILES:</b>	CCCCNCCC#N
<b>Mol. weight [g/mol]:</b>	126.20
<b>CAS:</b>	693-51-6

## Physical Properties

Property code	Value	Unit	Source
gf	230.63	kJ/mol	Joback Method
hf	30.54	kJ/mol	Joback Method
hfus	20.49	kJ/mol	Joback Method
hvap	48.09	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.290		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
tb	511.81	K	Joback Method
tc	701.21	K	Joback Method
tf	286.30	K	Joback Method
vc	0.488	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.36	J/mol×K	511.81	Joback Method
cpg	283.35	J/mol×K	543.38	Joback Method
cpg	293.85	J/mol×K	574.94	Joback Method
cpg	303.86	J/mol×K	606.51	Joback Method
cpg	313.40	J/mol×K	638.07	Joback Method
cpg	322.48	J/mol×K	669.64	Joback Method
cpg	331.13	J/mol×K	701.21	Joback Method

# Sources

<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=C693516&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C693516&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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