

# N-n-Butylpropionamide

<b>Other names:</b>	N-Butylpropanamide Propanamide, N-butyl-
<b>Inchi:</b>	InChI=1S/C7H15NO/c1-3-5-6-8-7(9)4-2/h3-6H2,1-2H3,(H,8,9)
<b>InchiKey:</b>	XQZDWKBCGAJXLC-UHFFFAOYSA-N
<b>Formula:</b>	C7H15NO
<b>SMILES:</b>	CCCCNC(=O)CC
<b>Mol. weight [g/mol]:</b>	129.20
<b>CAS:</b>	2955-67-1

## Physical Properties

Property code	Value	Unit	Source
gf	-31.47	kJ/mol	Joback Method
hf	-246.92	kJ/mol	Joback Method
hfus	20.58	kJ/mol	Joback Method
hvap	44.36	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.313		Crippen Method
mcvol	121.040	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	1140.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1140.00		NIST Webbook
tb	463.60	K	Joback Method
tc	643.92	K	Joback Method
tf	271.24	K	Joback Method
vc	0.469	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.27	J/mol×K	463.60	Joback Method
cpg	271.21	J/mol×K	493.65	Joback Method
cpg	282.64	J/mol×K	523.71	Joback Method

cpg	293.59	J/mol×K	553.76	Joback Method
cpg	304.06	J/mol×K	583.82	Joback Method
cpg	314.06	J/mol×K	613.87	Joback Method
cpg	323.61	J/mol×K	643.92	Joback Method

## 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=C2955671&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2955671&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>rinpola:</b>	Non-polar retention indices
<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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