

# 1-Butanamine, N-butyl-N-nitro-

<b>Other names:</b>	Dibutylamine, N-nitro- Dibutylnitramine N-Nitrodibutylamine Di-n-butylnitramine
<b>Inchi:</b>	InChI=1S/C8H18N2O2/c1-3-5-7-9(10(11)12)8-6-4-2/h3-8H2,1-2H3
<b>InchiKey:</b>	IBFAEPSQNZNTBK-UHFFFAOYSA-N
<b>Formula:</b>	C8H18N2O2
<b>SMILES:</b>	CCCCN(CCCC)[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	174.24
<b>CAS:</b>	4164-31-2

## Physical Properties

Property code	Value	Unit	Source
chl	-5510.70	kJ/mol	NIST Webbook
gf	162.81	kJ/mol	Joback Method
hf	-151.68	kJ/mol	Joback Method
hfus	30.86	kJ/mol	Joback Method
hvap	52.04	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.080		Crippen Method
mcvol	150.980	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
tb	546.72	K	Joback Method
tc	740.57	K	Joback Method
tf	356.00	K	Joback Method
vc	0.584	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.10	J/molxK	546.72	Joback Method
cpg	387.42	J/molxK	579.03	Joback Method
cpg	400.99	J/molxK	611.34	Joback Method
cpg	413.85	J/molxK	643.65	Joback Method

cpg	426.02	J/mol×K	675.96	Joback Method
cpg	437.52	J/mol×K	708.27	Joback Method
cpg	448.40	J/mol×K	740.57	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=C4164312&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4164312&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>chl:</b>	Standard liquid enthalpy of combustion
<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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