

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

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4164312&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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