

1-Butanamine, N-methyl-N-nitroso-

Other names:	Butylmethylnitrosamine Butylamine, N-methyl-N-nitroso- Methylbutylnitrosamine N-Methyl-N-butylnitrosamine N-Methyl-N-nitrosobutylamine Butanamine, N-methyl-N-nitroso- MBNA Methyl-butyl-nitrosamin Methyl-n-butylnitrosamine N-Nitroso-n-butylmethyamine Nitrosomethyl-n-butylamine N-Nitrosomethyl-N-butylamine N-Nitroso-N-methyl-N-n-butylamine NMBA N-Butyl-N-methylnitrosamine N-Nitroso-N-methylbutylamine
Inchi:	InChI=1S/C5H12N2O/c1-3-4-5-7(2)6-8/h3-5H2,1-2H3
InchiKey:	PKTSCJXWLVREKX-UHFFFAOYSA-N
Formula:	C5H12N2O
SMILES:	CCCCN(C)N=O
Mol. weight [g/mol]:	116.16
CAS:	7068-83-9

Physical Properties

Property code	Value	Unit	Source
hf	-247.19	kJ/mol	Joback Method
hvap	37.86	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.400		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
tb	389.64	K	Joback Method
tc	556.16	K	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7068839&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf:	Enthalpy of formation 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

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