

1-Butanol, 4-(butylnitrosoamino)-

Other names:	1-Butanol, 4-(butylnitrosamino)- Butyl(4-hydroxybutyl)nitrosamine Butylbutanolnitrosamine N-Butyl-N-(4-hydroxybutyl)nitrosamine BBN Butanol (4)-butyl-nitrosamine Butyl-butanol(4)-nitrosamin n-Butyl-(4-hydroxybutyl)nitrosamine 4-(Butylnitrosamino)-1-butanol 4-(n-Butylnitrosamino)-1-butanol Dibutylamine, 4-hydroxy-N-nitroso- 4-Hydroxybutylbutylnitrosamine N-Nitroso-n-butyl-(4-hydroxybutyl)amine
Inchi:	InChI=1S/C8H18N2O2/c1-2-3-6-10(9-12)7-4-5-8-11/h11H,2-8H2,1H3
InchiKey:	DIKPQFXYECAYPC-UHFFFAOYSA-N
Formula:	C8H18N2O2
SMILES:	CCCCN(CCCCO)N=N
Mol. weight [g/mol]:	174.24
CAS:	3817-11-6

Physical Properties

Property code	Value	Unit	Source
hf	-461.34	kJ/mol	Joback Method
hvap	61.22	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.542		Crippen Method
mcvol	150.980	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
tb	550.46	K	Joback Method
tc	710.58	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=C3817116&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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