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=O
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

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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

Latest version available from:
https://www.chemeo.com/cid/64-528-5/1-Butanol-4-butylnitrosoamino.pdf
Generated by Cheméo on 2025-12-06 03:48:49.837307038 +0000 UTC m=+4741127.367347702.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.