1-Butanamine, N-butyl-N-nitroso-

Other names:	Dibutylamine, N-nitroso-
	Dibutylnitrosoamine
	N-Nitrosodi-N-butylamine
	N-Nitrosodibutylamine
	Nitrosodibutylamine
	N-di-n-Butylnitrosoamine
	Butylamine, N-nitrosodi-
	Di-N-butylnitrosamin
	Di-N-butylnitrosoamine
	DBNA
	N-Butyl-N-nitroso-1-butamine
	N-Butyl-N-nitroso-1-butaneamine
	N,N-Di-n-butylnitrosamine
	N,N-Dibutylnitrosoamine
	Nitrosodi-N-butylamine
	NDBA
	Dibutylnitrosamine
	Di-n-butylnitrosamine
	Rcra waste number U172
	N-Butyl-N-nitroso-1-butanamine
	N-butyl-N-nitrosobutanamine
	N,N-Dibutylnitrosamine
	NSC 6830
	Benzenamine, 3-methyl, mono-TMS
Inchi:	InChI=1S/C8H18N2O/c1-3-5-7-10(9-11)8-6-4-2/h3-8H2,1-2H3
InchiKey:	YGJHZCLPZAZIHH-UHFFFAOYSA-N
Formula:	C8H18N2O
SMILES:	CCCCN(CCCC)N=O
Mol. weight [g/mol]:	158.24
CAS:	924-16-3

Physical Properties

Property code	Value	Unit	Source
hf	-309.11	kJ/mol	Joback Method
hvap	44.54	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method

logp	2.570		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	213.63		NIST Webbook
rinpol	215.35		NIST Webbook
rinpol	213.63		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1269.00		NIST Webbook
ripol	1691.00		NIST Webbook
ripol	1722.00		NIST Webbook
ripol	1722.00		NIST Webbook
tb	458.28	K	Joback Method
tc	622.63	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=C924163&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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

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