

1-Butanamine, N-ethyl-N-nitroso-

Other names:	Butylamine, N-ethyl-N-nitroso- N-Butyl-N-ethylnitrosamine N-Ethyl-N-nitrosobutylamine N-Nitrosoethyl-N-butylamine Aethyl-N-butyl-nitrosoamin Butanamine, N-ethyl-N-nitroso- Ethyl-N-butylnitrosamine N-Nitroso-N-butylethylamine Nitrosoethylbutylamine Butylethylnitrosamin N-Ethyl-N-butylnitrosamine NSC 135
Inchi:	InChI=1S/C6H14N2O/c1-3-5-6-8(4-2)7-9/h3-6H2,1-2H3
InchiKey:	ZGMCNGHHUQZNIH-UHFFFAOYSA-N
Formula:	C6H14N2O
SMILES:	CCCCN(CC)N=O
Mol. weight [g/mol]:	130.19
CAS:	4549-44-4

Physical Properties

Property code	Value	Unit	Source
hf	-267.83	kJ/mol	Joback Method
hvap	40.09	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.790		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
tb	412.52	K	Joback Method
tc	578.47	K	Joback Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4549444&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

hf: Enthalpy of formation at standard conditions
h_{vap}: Enthalpy of vaporization at standard conditions
log₁₀ws: Log₁₀ of Water solubility in mol/l
log_p: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature

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