

Benzenemethanamine, N-nitroso-N-phenyl-

Other names:	Benzylamine, N-nitroso-N-phenyl- Benzylphenylnitrosamine N-Benzyl-N-nitrosoaniline N-Phenyl-N-nitrosobenzylamine N-Nitrosophenylbenzylamine N-Nitroso-N-phenyl-benzylamine
Inchi:	InChI=1S/C13H12N2O/c16-14-15(13-9-5-2-6-10-13)11-12-7-3-1-4-8-12/h1-10H,11H2
InchiKey:	BCIBCBXFXGKGBL-UHFFFAOYSA-N
Formula:	C13H12N2O
SMILES:	O=NN(Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	212.25
CAS:	612-98-6

Physical Properties

Property code	Value	Unit	Source
hf	60.75	kJ/mol	Joback Method
hvap	60.22	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.375		Crippen Method
mcvol	168.040	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
tb	626.04	K	Joback Method
tc	858.75	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C612986&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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