

Benzene, 1-methyl-4-nitroso-

Other names:	Toluene, p-nitroso- p-Methylnitrosobenzene p-Nitrosotoluene 1-Methyl-4-nitrosobenzene 4-Nitrosotoluene 4-Methylnitrosobenzene
Inchi:	InChI=1S/C7H7NO/c1-6-2-4-7(8-9)5-3-6/h2-5H,1H3
InchiKey:	NYJYFSGMYHSTNZ-UHFFFAOYSA-N
Formula:	C7H7NO
SMILES:	<chem>Cc1ccc(N=O)cc1</chem>
Mol. weight [g/mol]:	121.14
CAS:	623-11-0

Physical Properties

Property code	Value	Unit	Source
hf	-130.94	kJ/mol	Joback Method
hvap	43.21	kJ/mol	Joback Method
ie	8.80 ± 0.10	eV	NIST Webbook
log10ws	-2.71		Crippen Method
logp	2.393		Crippen Method
mcvol	97.280	ml/mol	McGowan Method
pc	3945.61	kPa	Joback Method
tb	454.62	K	Joback Method
tc	666.63	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C623110&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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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