

Benzene, 1-methyl-2-nitroso-

Other names:	Toluene, o-nitroso- o-Methylnitrosobenzene o-Nitrosotoluene 1-Methyl-2-nitrosobenzene 2-Methyl-1-nitrosobenzene 2-Nitrosotoluene Nitrosotoluene
Inchi:	InChI=1S/C7H7NO/c1-6-4-2-3-5-7(6)8-9/h2-5H,1H3
InchiKey:	TWLBRQVYXPMCFK-UHFFFAOYSA-N
Formula:	C7H7NO
SMILES:	Cc1ccccc1N=O
Mol. weight [g/mol]:	121.14
CAS:	611-23-4

Physical Properties

Property code	Value	Unit	Source
hf	-130.94	kJ/mol	Joback Method
hvap	43.21	kJ/mol	Joback Method
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

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=C611234&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ 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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