

N-METHYL-N'-NITROGUANIDINE

Other names:	1-Methyl-3-nitroguanidine Guanidine, N-methyl-N'-nitro- Guanidine, 1-methyl-3-nitro- N-methyl-N''-nitroguanidine
Inchi:	InChI=1S/C2H6N4O2/c1-4-2(3)5-6(7)8/h1H3,(H3,3,4,5)
InchiKey:	XCXKNNGWSDYMMMS-UHFFFAOYSA-N
Formula:	C2H6N4O2
SMILES:	CN/C(N)=N/[N+](=O)[O-]
Mol. weight [g/mol]:	118.10

Physical Properties

Property code	Value	Unit	Source
chs	-1576.00	kJ/mol	NIST Webbook
logp	-1.288		Crippen Method
mcvol	82.100	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4245765&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

chs:	Standard solid enthalpy of combustion
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/48-146-7/N-METHYL-N-NITROGUANIDINE.pdf>

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