

Imidazole, 4-methyl-5-nitro-

Other names:	Imidazole, 4-methyl-5-nitro- 4-Methyl-5-nitroimidazole 5-Methyl-4-nitroimidazole Imidazole, 5-methyl-4-nitro- 4-Methyl-5-nitro-1H-imidazole Imidazole, 4(or 5)-methyl-5(or 4)-nitro-
Inchi:	InChI=1S/C4H5N3O2/c1-3-4(7(8)9)6-2-5-3/h2H,1H3,(H,5,6)
InchiKey:	WSYOWIMKNNMEMZ-UHFFFAOYSA-N
Formula:	C4H5N3O2
SMILES:	<chem>Cc1nc[nH]c1[N+](=O)[O-]</chem>
Mol. weight [g/mol]:	127.10

Physical Properties

Property code	Value	Unit	Source
logp	0.144		Crippen Method
mcvol	85.140	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C14003668&Units=SI>

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.cheméo.com/cid/30-872-0/Imidazole-4-methyl-5-nitro.pdf>

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