

Imidazole-5-carbonitrile, 1-methyl-4-nitro-

Inchi:	InChI=1S/C5H4N4O2/c1-8-3-7-5(9(10)11)4(8)2-6/h3H,1H3
InchiKey:	LXXDMPXVEZYDCI-UHFFFAOYSA-N
Formula:	C5H4N4O2
SMILES:	Cn1cnc([N+](=O)[O-])c1C#N
Mol. weight [g/mol]:	152.11
CAS:	40648-96-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	0.200		Crippen Method
mcvol	100.610	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40648962&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/120-293-3/Imidazole-5-carbonitrile-1-methyl-4-nitro.pdf>

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