

# Imidazole-5(4)-carboxamide, n-methyl-4(5)-nitro-

Inchi:	InChI=1S/C5H6N4O3/c1-6-5(10)3-4(9(11)12)8-2-7-3/h2H,1H3,(H,6,10)(H,7,8)
InchiKey:	FSFYGQQWENXEBS-UHFFFAOYSA-N
Formula:	C5H6N4O3
SMILES:	CN=C(O)c1nc[nH]c1[N+](=O)[O-]
Mol. weight [g/mol]:	170.13
CAS:	57445-42-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.00		Crippen Method
logp	-0.230		Crippen Method
mcvol	110.780	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C57445428&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C57445428&amp;Units=SI</a>

## Legend

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

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