

Imidazole, 1-methyl-5-(methylsulfonyl)-4-nitro-

Inchi:	InChI=1S/C5H7N3O4S/c1-7-3-6-4(8(9)10)5(7)13(2,11)12/h3H,1-2H3
InchiKey:	PARSHOLGHQRIIZ-UHFFFAOYSA-N
Formula:	C5H7N3O4S
SMILES:	Cn1cnc([N+](=O)[O-])c1S(C)(=O)=O
Mol. weight [g/mol]:	205.19
CAS:	13755-79-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.87		Crippen Method
logp	-0.268		Crippen Method
mcvol	127.320	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=C13755798&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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