

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

Inchi:	InChI=1S/C4H5N3O4S/c1-12(10,11)4-3(7(8)9)5-2-6-4/h2H,1H3,(H,5,6)
InchiKey:	AGOXDXWPTKSCRO-UHFFFAOYSA-N
Formula:	C4H5N3O4S
SMILES:	CS(=O)(=O)c1[nH]cnc1[N+](=O)[O-]
Mol. weight [g/mol]:	191.16
CAS:	110299-87-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.80		Crippen Method
logp	-0.760		Crippen Method
mcvol	113.230	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110299871&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/96-670-2/Imidazole-5-methylsulfonyl-4-nitro.pdf>

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