

# Imidazole, 4-nitro-5-(propylsulfonyl)-

<b>Inchi:</b>	InChI=1S/C6H9N3O4S/c1-2-3-14(12,13)6-5(9(10)11)7-4-8-6/h4H,2-3H2,1H3,(H,7,8)
<b>InchiKey:</b>	XUTRKPWAVOXOO-UHFFFAOYSA-N
<b>Formula:</b>	C6H9N3O4S
<b>SMILES:</b>	CCCS(=O)(=O)c1[nH]cnc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	219.22
<b>CAS:</b>	99980-28-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.64		Crippen Method
logp	0.020		Crippen Method
mcvol	141.410	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C99980286&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C99980286&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

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

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