

# N-(Mesitylenesulfonyl)imidazole

<b>Other names:</b>	1-(2-Mesitylenesulfonyl)imidazole Mesitylenesulfonyl-1-imidazole Mesitylenesulfonylimidazole 1-(Mesitylene-2-sulfonyl)imidazole 1H-Imidazole, 1-[(2,4,6-trimethylphenyl)sulfonyl]- 1-[(2,4,6-trimethylphenyl)sulphonyl]-1H-imidazole
<b>Inchi:</b>	InChI=1S/C12H14N2O2S/c1-9-6-10(2)12(11(3)7-9)17(15,16)14-5-4-13-8-14/h4-8H,1-3H
<b>InchiKey:</b>	XFHVQSPNDDOABS-UHFFFAOYSA-N
<b>Formula:</b>	C12H14N2O2S
<b>SMILES:</b>	<chem>Cc1cc(C)c(S(=O)(=O)n2ccnc2)c(C)c1</chem>
<b>Mol. weight [g/mol]:</b>	250.32
<b>CAS:</b>	50257-39-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Crippen Method
logp	2.045		Crippen Method
mcvol	184.770	ml/mol	McGowan Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C50257391&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C50257391&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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