

# 1-(2-Mesitylenesulfonyl)-1,2,4-triazole

<b>Other names:</b>	N-Mesitylenesulfonyl-1,2,4-triazole Mesitylenesulfonyl-1H-1,2,4-triazole 1-(2-Mesitylsulfonyl)-1H-1,2,4-triazole 1H-1,2,4-Triazole, 1-[(2,4,6-trimethylphenyl)sulfonyl]- mesityl 1,2,4-triazole-1-sulphonate
<b>Inchi:</b>	InChI=1S/C11H13N3O2S/c1-8-4-9(2)11(10(3)5-8)17(15,16)14-7-12-6-13-14/h4-7H,1-3H3
<b>InchiKey:</b>	XNKYPZJMRHXJJQ-UHFFFAOYSA-N
<b>Formula:</b>	C11H13N3O2S
<b>SMILES:</b>	<chem>Cc1cc(C)c(S(=O)(=O)n2cncn2)c(C)c1</chem>
<b>Mol. weight [g/mol]:</b>	251.31
<b>CAS:</b>	54230-59-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.38		Crippen Method
logp	1.440		Crippen Method
mcvol	180.660	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=C54230590&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C54230590&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>

## 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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