N-Mesitylenesulphonylimidazole

Other names:	1-(2-Mesitylenesulfonyl)imidazole
	1-(Mesitylene-2-sulfonyl)imidazole
	1-[(2,4,6-trimethylphenyl)sulphonyl]-1H-imidazole
	1H-Imidazole, 1-[(2,4,6-trimethylphenyl)sulfonyl]-
	Mesitylenesulfonyl-1-imidazole
	Mesitylenesulfonylimidazole
Inchi:	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
InchiKey:	XFHVQSPNDDOABS-UHFFFAOYSA-N
Formula:	C12H14N2O2S
SMILES:	Cc1cc(C)c(S(=O)(=O)n2ccnc2)c(C)c1
Mol. weight [g/mol]:	250.32

Physical Properties

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

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50257391&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume