

1-(2,4,6-Trisopropylbenzenesulfonyl)imidazole

Other names:	N-(2,4,6-Triisopropylbenzenesulfonyl)imidazole 1-(2,4,6-Triisopropylbenzene sulfonyl)-imidazole 1H-Imidazole, 1-[[2,4,6-tris(1-methylethyl)phenyl]sulfonyl]- Imidazole, 1-[2,4,6-tris(1-methylethyl)phenylsulfonyl]- 1-(2',4',6'-triisopropylbenzenesulphonyl)imidazole
Inchi:	InChI=1S/C18H26N2O2S/c1-12(2)15-9-16(13(3)4)18(17(10-15)14(5)6)23(21,22)20-8-7-1
InchiKey:	AGGRGODMKWLSDE-UHFFFAOYSA-N
Formula:	C18H26N2O2S
SMILES:	CC(C)c1cc(C(C)C)c(S(=O)(=O)n2ccnc2)c(C(C)C)c1
Mol. weight [g/mol]:	334.48
CAS:	50257-40-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.74		Crippen Method
logp	4.490		Crippen Method
mcvol	269.310	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=C50257404&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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