

tert-Butyldimethylsilyl 4-methylbenzenesulfonate

Inchi: InChI=1S/C13H22O3SSi/c1-11-7-9-12(10-8-11)17(14,15)16-18(5,6)13(2,3)4/h7-10H,1-6H
InchiKey: PHMOKJCOHPBPSS-UHFFFAOYSA-N
Formula: C13H22O3SSi
SMILES: Cc1ccc(S(=O)(=O)O[Si](C)(C)C(C)(C)C)cc1
Mol. weight [g/mol]: 286.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.86		Crippen Method
logp	3.706		Crippen Method
rinpol	1866.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U373380&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/63-978-7/tert-Butyldimethylsilyl-4-methylbenzenesulfonate.pdf>

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