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