

N-(2-Hydroxy-propionyl)-4-methyl-benzenesulfonamide-N,O-di(tert.-butyldimethylsilyl)-

InChIKey:

InChI=1S/C22H41NO4SSi2/c1-17-13-15-19(16-14-17)28(25,26)23(29(9,10)21(3,4)5)20(21)1-2/SZLRXHXMUJSJ-UHFFFAOYSA-N

Formula: C22H41NO4SSi2

SMILES: Cc1ccc(S(=O)(=O)N(C(=O)C(C)O[Si](C)(C)C(C)(C)C)[Si](C)(C)C(C)(C)C)cc1

Mol. weight [g/mol]: 471.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.14		Crippen Method
logp	5.928		Crippen Method
rinpol	2532.00		NIST Webbook

Sources

- Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
- Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
- NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U374398&Units=SI>

Legend

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

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