N-(2-Hydroxy-propionyl)-4-methyl-benzenesulfona O-trimethylsilyl-

Inchi: InChI=1S/C13H21NO4SSi/c1-10-6-8-12(9-7-10)19(16,17)14-13(15)11(2)18-20(3,4)5/h6-9

InchiKey: BPKWNNTYFHUBIR-UHFFFAOYSA-N

Formula: C13H21NO4SSi

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

Mol. weight [g/mol]: 315.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.94		Crippen Method
logp	2.040		Crippen Method
rinpol	2076.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374820&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices