

Benzenesulfonamide, 4-chloro, N-trimethylsilyl-N-butyryl-

Inchi: InChI=1S/C13H20ClNO3SSi/c1-5-6-13(16)15(20(2,3)4)19(17,18)12-9-7-11(14)8-10-12/h

InchiKey: DVBRHKHDOJTTRE-UHFFFAOYSA-N

Formula: C13H20ClNO3SSi

SMILES: CCCC(=O)N([Si](C)(C)C)S(=O)(=O)c1ccc(Cl)cc1

Mol. weight [g/mol]: 333.91

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Crippen Method
logp	3.492		Crippen Method
rinpol	2035.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U374376&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

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/44-626-8/Benzenesulfonamide-4-chloro-N-trimethylsilyl-N-butyryl.pdf>

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