

N-(2-Bromobutyl)-4-chloro-benzenesulfonamide

N-trimethylsilyl-

InChI=1S/C13H19BrClNO3SSi/c1-5-12(14)13(17)16(21(2,3)4)20(18,19)11-8-6-10(15)7-9

InchiKey: KFWLESIQRUUKNF-UHFFFAOYSA-N

Formula: C13H19BrClNO3SSi

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

Mol. weight [g/mol]: 412.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.29		Crippen Method
logp	3.866		Crippen Method
rinpol	2188.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U374373&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

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