

N-(3-Bromo-4-hydroxy-phenyl)-4-nitro-benzenesulfonamide-N,O-di(trimethylsilyl)-

InChIKey:

InChI=1S/C18H25BrN2O5SSi2/c1-28(2,3)21(15-9-12-18(17(19)13-15)26-29(4,5)6)27(24)28

Formula:

C18H25BrN2O5SSi2

SMILES:

C[Si](C)(C)Oc1ccc(N([Si](C)(C)C)S(=O)(=O)c2ccc([N+](=O)[O-])cc2)cc1Br

Mol. weight [g/mol]:

517.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.59		Crippen Method
logp	5.601		Crippen Method
rinpol	2847.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U374410&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.cheméo.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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