

3-Nitrobenzoic acid, tert-butyldimethylsilyl ester

Other names: Benzoic acid, 3-nitro-, tert-butyldimethylsilyl ester

3-Nitrobenzoic acid BDMS

Inchi: InChI=1S/C13H19NO4Si/c1-13(2,3)19(4,5)18-12(15)10-7-6-8-11(9-10)14(16)17/h6-9H,1

InchiKey: GJZBAVMSSINKTD-UHFFFAOYSA-N

Formula: C13H19NO4Si

SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1cccc([N+](=O)[O-])c1

Mol. weight [g/mol]: 281.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.51		Crippen Method
logp	3.757		Crippen Method
rinpol	1860.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U373105&Units=SI>

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

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/39-125-0/3-Nitrobenzoic-acid-tert-butyldimethylsilyl-ester.pdf>

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