

o-Aminobenzoic acid, N-isoBOC TBDMS

Inchi: InChI=1S/C18H29NO4Si/c1-13(2)12-22-17(21)19-15-11-9-8-10-14(15)16(20)23-24(6,7)1
InchiKey: PTXBZJWBHDUQPBUHFFFAOYSA-N
Formula: C18H29NO4Si
SMILES: CC(C)COC(=O)Nc1ccccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 351.51

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -3.14 | | Crippen Method |
| logp | 5.053 | | Crippen Method |
| rinpol | 2211.00 | | NIST Webbook |
| rinpol | 2211.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R260629&Units=SI>

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/123-063-5/o-Aminobenzoic-acid-N-isoBOC-TBDMS.pdf>

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