

4-Aminobenzoic acid, N-(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester

Other names: Benzoic acid, 4-amino, TBDMS
Inchi: InChI=1S/C₁₉H₃₅N₂O₂Si₂/c1-18(2,3)23(7,8)20-16-13-11-15(12-14-16)17(21)22-24(9,10)
InchiKey: MWRAWVXPRARZSM-UHFFFAOYSA-N
Formula: C₁₉H₃₅NO₂Si₂
SMILES: CC(C)(C)[Si](C)(C)Nc1ccc(C(=O)O[Si](C)(C)C(C)(C)C)cc1
Mol. weight [g/mol]: 365.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.01		Crippen Method
logp	6.266		Crippen Method
rinpol	1850.00		NIST Webbook
rinpol	1850.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U364387&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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