

3-Hydroxyphenylacetic acid, O-(tert-butyl dimethylsilyl)-, tert-butyl dimethylsilyl ester

Other names: tert-Butyl(dimethyl)silyl 3-hydroxyphenylacetate
3-Hydroxyphenylacetic acid, TBDMS

3-Hydroxyphenylacetic acid, 2tdms derivative

Inchi: InChI=1S/C20H36O3Si2/c1-19(2,3)24(7,8)22-17-13-11-12-16(14-17)15-18(21)23-25(9,10)

InchiKey: QDRQCMKSFYJFRJ-UHFFFAOYSA-N

Formula: C20H36O3Si2

SMILES: CC(C)(C)[Si](C)(C)OC(=O)Cc1ccc(O[Si](C)(C)C(C)(C)C)c1

Mol. weight [g/mol]: 380.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.96		Crippen Method
logp	6.161		Crippen Method
rinpol	2063.00		NIST Webbook
rinpol	2064.00		NIST Webbook
rinpol	2063.00		NIST Webbook
rinpol	2064.00		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=U332869&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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