3-Hydroxyphenylacetic acid, O-(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester

Other names: tert-Butyl(dimethyl)silyl [3-pyrrol[tert-butyl(dimethyl)silyl]oxymorphophenyl)acetate
3-Hydroxyphenylacetic acid, TBDMS
3-Hydroxyphenylacetic acid, 2tbdms 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)Cc1cccc(O[Si](C)(C)C(C)(C)C)c1

Mol. weight [g/mol]: 380.68

Physical Properties

Property code	Value	Unit	Source
logp	6.162		Crippen Method
rinpol	2063.00		NIST Webbook
rinpol	2064.00		NIST Webbook
rinpol	2063.00		NIST Webbook
rinpol	2064.00		NIST Webbook
tb	600.63	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U332869&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature

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