

2,4-Dihydroxybenzoic acid, bis(tert-butyl dimethylsilyl) ether, tert-butyl dimethylsilyl ester

Other names: «beta»-Resorcylic acid, DMTBS
«beta»-Resorcylic acid, TBDMS

2,4-Dihydroxybenzoic acid, 3tbdms derivative

Inchi: InChI=1S/C25H48O4Si3/c1-23(2,3)30(10,11)27-19-16-17-20(22(26)29-32(14,15)25(7,8)9

InchiKey: SPLDOCOKVQMIQC-UHFFFAOYSA-N

Formula: C25H48O4Si3

SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccc(O[Si](C)(C)C(C)(C)C)cc1O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 496.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	8.617		Crippen Method
rinpol	2439.20		NIST Webbook
rinpol	2483.00		NIST Webbook
rinpol	2484.00		NIST Webbook
rinpol	2439.20		NIST Webbook
rinpol	2483.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U352816&Units=SI>

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

Crippen Method: https://www.chemeo.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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