

Gentisic acid, O,O'-bis(tert-butyl dimethylsilyl)-, tert-butyl dimethylsilyl ester

Other names: tert-Butyl(dimethyl)silyl 2,5-bispyrrolidone tert-butyl(dimethyl)silyloxymorphobenzoate
Gentisic acid, DMTBS

2,5-Dihydroxybenzoic acid, 3tdms derivative

Inchi: InChI=1S/C25H48O4Si3/c1-23(2,3)30(10,11)27-19-16-17-21(28-31(12,13)24(4,5)6)20(18)

InchiKey: VUDPIPZFGUHBPG-UHFFFAOYSA-N

Formula: C25H48O4Si3

SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1cc(O[Si](C)(C)C(C)(C)C)ccc1O[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 | 2421.10 | | NIST Webbook |
| rinpol | 2450.00 | | NIST Webbook |
| rinpol | 2450.00 | | NIST Webbook |
| rinpol | 2421.10 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U332902&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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