

Glycine, N-[4-[(trimethylsilyl)oxy]benzoyl]-, trimethylsilyl ester

Other names:

4-Hydroxyhippuric acid, di-TMS

Glycine, N-(4-hydroxybenzoyl)-, bis(trimethylsilyl) deriv.

Hippuric acid, 4-hydroxy, bis-TMS

Hippuric acid, 4-hydroxy, TMS, # 2

Inchi: InChI=1S/C15H25NO4Si2/c1-21(2,3)19-13-9-7-12(8-10-13)15(18)16-11-14(17)20-22(4,5

InchiKey: FSRUVIACJHADSP-UHFFFAOYSA-N

Formula: C15H25NO4Si2

SMILES: C[Si](C)(C)OC(=O)CNC(=O)c1ccc(O[Si](C)(C)C)cc1

Mol. weight [g/mol]: 339.53

CAS: 55622-53-2

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 0.59 | | Crippen Method |
| logp | 3.008 | | Crippen Method |
| rinpol | 2190.00 | | NIST Webbook |
| rinpol | 2202.00 | | NIST Webbook |
| rinpol | 2192.00 | | NIST Webbook |
| rinpol | 2202.00 | | NIST Webbook |
| rinpol | 2233.00 | | NIST Webbook |
| rinpol | 2239.00 | | NIST Webbook |
| rinpol | 2202.00 | | NIST Webbook |

Sources

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

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55622532&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/30-633-5/Glycine-N-4-trimethylsilyl-oxy-benzoyl-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-24 16:17:54.636263551 +0000 UTC m=+16264723.556840867.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.