

Glycine, N-(trimethylsilyl)-N-[2-[(trimethylsilyl)oxy]benzoyl] trimethylsilyl ester

Other names: 2-Hydroxyhippuric acid, N,O,O-tris(trimethylsilyl) deriv.

2-Hydroxyhippuric acid, tris-TMS

2-Hydroxyhippuric acid, 3tms derivative

Inchi: InChI=1S/C18H33NO4Si3/c1-24(2,3)19(14-17(20)23-26(7,8)9)18(21)15-12-10-11-13-16(

InchiKey: SJLWAPOSGSUWJU-UHFFFAOYSA-N

Formula: C18H33NO4Si3

SMILES: C[Si](C)(C)OC(=O)CN(C(=O)c1ccccc1O[Si](C)(C)C)[Si](C)(C)C

Mol. weight [g/mol]: 411.72

CAS: 55517-53-8

Physical Properties

Property code	Value	Unit	Source
log10ws	1.90		Crippen Method
logp	4.556		Crippen Method
rinsol	1954.00		NIST Webbook
rinsol	1954.00		NIST Webbook
rinsol	1954.00		NIST Webbook
rinsol	1954.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55517538&Units=SI>

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinsol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/56-737-2/Glycine-N-trimethylsilyl-N-2-trimethylsilyl-oxy-benzoyl-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-24 11:09:11.532709749 +0000 UTC m=+16246200.453287062.

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