

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

Other names:

o-Trimethylsilyloxyhippuric acid, trimethylsilyl ester
2-Trimethylsilyloxyhippuric acid, trimethylsilyl ester
2-Hydroxyhippuric acid, bis-TMS
2-Hydroxyhippuric acid, di-TMS
2-Hydroxyhippuric acid, trimethylsilyl ether, trimethylsilyl ester
2-Hydroxyhippuric acid, 2tms derivative

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

InchiKey: YWJABPMELDZKDW-UHFFFAOYSA-N

Formula: C15H25NO4Si2

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

Mol. weight [g/mol]: 339.53

CAS: 55887-56-4

Physical Properties

Property code	Value	Unit	Source
log10ws	0.59		Crippen Method
logp	3.008		Crippen Method
rinpol	2086.00		NIST Webbook
rinpol	2087.00		NIST Webbook
rinpol	2048.00		NIST Webbook
rinpol	2047.00		NIST Webbook
rinpol	2047.00		NIST Webbook
rinpol	2046.00		NIST Webbook
rinpol	2075.80		NIST Webbook
rinpol	2047.00		NIST Webbook
rinpol	2075.80		NIST Webbook

Sources

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

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55887564&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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