

# Glycine, N-benzoyl-N-(trimethylsilyl)-, trimethylsilyl ester

Other names:

Hippuric acid, diTMS  
Hippuric acid (2TMS)  
Hippuric acid, N-trimethylsilyl-, trimethylsilyl ester  
Hippuric acid (TMS)  
Hippuric acid, 2tms derivative

Inchi:

InChI=1S/C15H25NO3Si2/c1-20(2,3)16(12-14(17)19-21(4,5)6)15(18)13-10-8-7-9-11-13/1

InchiKey:

ISPSCQNROBRNPC-UHFFFAOYSA-N

Formula:

C15H25NO3Si2

SMILES:

C[Si](C)(C)OC(=O)CN(C(=O)c1ccccc1)[Si](C)(C)C

Mol. weight [g/mol]:

323.53

CAS:

55133-85-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.91		Crippen Method
logp	3.342		Crippen Method
rinpol	1820.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1789.00		NIST Webbook
rinpol	1822.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1799.10		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1799.10		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1822.00		NIST Webbook

## Sources

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C55133852&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  
**rinpol:** Non-polar retention indices

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