

Glycine, N-benzoyl-, tert-butyldimethylsilyl ester

Other names:

Hippuric acid, tert-butyldimethylsilyl ester
tert-Butyl(dimethyl)silyl N-benzoylglycinate
Hippuric acid, DMTBS
Hippuric acid, tbdms derivative

Inchi:

InChI=1S/C15H23NO3Si/c1-15(2,3)20(4,5)19-13(17)11-16-14(18)12-9-7-6-8-10-12/h6-10

InchiKey:

AUAFREORTBXLPU-UHFFFAOYSA-N

Formula:

C15H23NO3Si

SMILES:

CC(C)(C)[Si](C)(C)OC(=O)CNC(=O)c1ccccc1

Mol. weight [g/mol]:

293.43

CAS:

105041-03-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.66		Crippen Method
logp	2.965		Crippen Method
rinpol	2113.60		NIST Webbook
rinpol	2095.00		NIST Webbook
rinpol	2113.60		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=C105041030&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/12-594-9/Glycine-N-benzoyl-tert-butyl-dimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-27 21:10:26.421246295 +0000 UTC m=+16541475.341823611.

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