

# 3-Amino-N-butyric acid, bis(trimethylsilyl) deriv.

<b>Other names:</b>	N,O-Bis-(trimethylsilyl)-3-aminobutyric acid 3-Aminobutyric acid, (2TMS)- 3-Aminobutyric acid, TMS 3-Aminobutyric acid, 2tms derivative
<b>Inchi:</b>	InChI=1S/C10H25NO2Si2/c1-9(11-14(2,3)4)8-10(12)13-15(5,6)7/h9,11H,8H2,1-7H3
<b>InchiKey:</b>	HPSBKFODWWCOSU-UHFFFAOYSA-N
<b>Formula:</b>	C10H25NO2Si2
<b>SMILES:</b>	CC(CC(=O)O[Si](C)(C)C)N[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	247.48
<b>CAS:</b>	58521-54-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	1.73		Crippen Method
logp	2.568		Crippen Method
rinpol	1223.00		NIST Webbook
rinpol	1223.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C58521543&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C58521543&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

Latest version available from:

<https://www.cheméo.com/cid/24-271-4/3-Amino-N-butyric-acid-bis-trimethylsilyl-deriv.pdf>

Generated by Cheméo on 2024-05-08 19:10:34.190888684 +0000 UTC m=+17484683.111466005.

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