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

Other names: N,O-Bis-(trimethylsilyl)-3-aminobutyric acid
3-Aminobutyric acid, (2TMS)-
3-Aminobutyric acid, TMS
3-Aminobutyric acid, 2tms derivative

Inchi: InChI=1S/C10H25NO2Si2/c1-9(11-14(2,3)4)8-10(12)13-15(5,6)7/h9,11H,8H2,1-7H3

InchiKey: HPSBKFODWWCOSU-UHFFFAOYSA-N

Formula: C10H25NO2Si2

SMILES: CC(CC(=O)O[Si](C)(C)C)N[Si](C)(C)C

Mol. weight [g/mol]: 247.48

CAS: 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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C58521543&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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