

3-Aminobutanoic acid, N-(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester

Other names: Butanoic acid, 3-[(tert-butyldimethylsilyl)amino]-, tert-butyldimethylsilyl ester, (±)-
Butanoic acid, 3-amino, O,N-bis-DMTBS

Inchi: InChI=1S/C16H37NO2Si2/c1-13(17-20(8,9)15(2,3)4)12-14(18)19-21(10,11)16(5,6)7/h13,
InchiKey: ZQDPBXJYXLAVEC-UHFFFAOYSA-N
Formula: C16H37NO2Si2
SMILES: CC(CC(=O)O[Si](C)(C)C(C)(C)C)N[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 331.64
CAS: 959109-26-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.79		Crippen Method
logp	4.908		Crippen Method
rinpol	1647.00		NIST Webbook
rinpol	1647.00		NIST Webbook

Sources

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

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C959109263&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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