

DL-3-Aminoisobutyric acid, N-(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester

Other names: tert-Butyl(dimethyl)silyl 3-((tert-butyldimethylsilyloxy)amino)propanoate, B-Aminoisobutyric acid, TBDMS

Inchi: InChI=1S/C16H37NO2Si2/c1-13(12-17-20(8,9)15(2,3)4)14(18)19-21(10,11)16(5,6)7/h13,14,15,16,17,18,19,20,21
InchiKey: WEIZCTOXVHJDFW-UHFFFAOYSA-N
Formula: C16H37NO2Si2
SMILES: CC(CN[Si](C)(C)C(C)(C)C)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 331.64
CAS: 959292-49-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.43		Crippen Method
logp	4.766		Crippen Method
rinpola	1643.70		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C959292490&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpola: Non-polar retention indices

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