

N-Acetyl-L-aspartic acid, N-(tert-butyldimethylsilyl)-, bis(tert-butyldimethylsilyl) ester

Other names:

N-Acetyl-L-aspartic acid, diTBS-MS

Inchi: InChI=1S/C24H51NO5Si3/c1-18(26)25(31(11,12)22(2,3)4)19(21(28)30-33(15,16)24(8,9)

InchiKey: CWTLUKMQFOTZND-UHFFFAOYSA-N

Formula: C24H51NO5Si3

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

Mol. weight [g/mol]: 517.92

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.20		Crippen Method
logp	6.696		Crippen Method
rinsol	2106.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U364324&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinsol: Non-polar retention indices

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