

L-Aspartic acid, N-(tert-butyldimethylsilyl)-, bis(tert-butyldimethylsilyl) ester

Other names:

Aspartic acid, triTBDMS

L-aspartic acid, 3tbdms derivative

Inchi:

InChI=1S/C22H49NO4Si3/c1-20(2,3)28(10,11)23-17(19(25)27-30(14,15)22(7,8)9)16-18(

InchiKey:

QQXNMPLNDTUYAN-QGZVFWFLSA-N

Formula:

C22H49NO4Si3

SMILES:

CC(C)(C)[Si](C)(C)NC(CC(=O)O[Si](C)(C)C(C)(C)C)C(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]:

475.89

CAS:

107715-96-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.21		Crippen Method
logp	6.437		Crippen Method
rinpol	2158.00		NIST Webbook
rinpol	2134.80		NIST Webbook
rinpol	2158.00		NIST Webbook
rinpol	2134.80		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C107715968&Units=SI>

Crippen Method:

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

Crippen Method:

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/12-444-5/L-Aspartic-acid-N-tert-butyldimethylsilyl-bis-tert-butyldimethylsilyl-ester.pdf>

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