

L-Threonine, N,O-bis(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester

Other names:

Thr, N,O,O-tris-TBDMS

Threonine tri-TBDMS

Thr, (3TBDMS)-

Thr, TBDMS

allo-Thr, TBDMS

L-threonine, 3tbdms derivative

Inchi: InChI=1S/C22H51NO3Si3/c1-17(25-28(13,14)21(5,6)7)18(23-27(11,12)20(2,3)4)19(24)2

InchiKey: DUARMRXEY AQNOD-ZWKOTPCHSA-N

Formula: C22H51NO3Si3

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

Mol. weight [g/mol]: 461.90

CAS: 107715-94-6

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -0.55 | | Crippen Method |
| logp | 6.909 | | Crippen Method |
| rinpol | 2029.00 | | NIST Webbook |
| rinpol | 2041.00 | | NIST Webbook |
| rinpol | 2029.00 | | NIST Webbook |

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C107715946&Units=SI>

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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