

Tyrosine, O-trimethylsilyl-, trimethylsilyl ester

Other names: Alanine, 3-[p-(trimethylsiloxy)phenyl]-, trimethylsilyl ester
Tyrosine, diTMS
Tyrosine, 2tms derivative

Inchi: InChI=1S/C15H27NO3Si2/c1-20(2,3)18-13-9-7-12(8-10-13)11-14(16)15(17)19-21(4,5)6/h

InchiKey: VQFWYFBDUJUQRW-UHFFFAOYSA-N

Formula: C₁₅H₂₇NO₃Si₂

SMILES: C[Si](C)(C)OC(=O)C(N)Cc1ccc(O[Si](C)(C)C)cc1

Mol. weight [g/mol]: 325.55

CAS: 7536-83-6

Physical Properties

Property code	Value	Unit	Source
log10ws	0.58		Crippen Method
logp	3.148		Crippen Method
rinsol	1901.00		NIST Webbook
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Sources

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

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C7536836&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinsol: Non-polar retention indices

Latest version available from:

<https://www.chemo.com/cid/15-226-4/Tyrosine-O-trimethylsilyl-trimethylsilyl-ester.pdf>

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