

L-Thyronine, trimethylsilyl ester

Other names: tert-Butyl(dimethyl)silyl o-(4-hydroxyphenyl)tyrosinate
Inchi: InChI=1S/C21H29NO4Si/c1-21(2,3)27(4,5)26-20(24)19(22)14-15-6-10-17(11-7-15)25-18
InchiKey: KNBGCMVLJMQKQR-UHFFFAOYSA-N
Formula: C₂₁H₂₉NO₄Si
SMILES: CC(C)(C)[Si](C)(C)OC(=O)C(N)Cc1ccc(Oc2ccc(O)cc2)cc1
Mol. weight [g/mol]: 387.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.85		Crippen Method
logp	4.603		Crippen Method
rinpol	2973.20		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U332755&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

Latest version available from:

<https://www.chemeo.com/cid/21-778-5/l-Thyronine-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-26 19:06:35.762146434 +0000 UTC m=+16447644.682723749.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.