

Pyrrolidin-2-one, 1-[1-(4-trimethylsilyloxycarbonylphenyl)butan-1-yl]-

Other names:

4,4-dimethyl-1-((alpha)-pyrrolidinobutyrophenone-M (carboxy-oxo-dihydro-)) diTMS ether

Inchi:

InChI=1S/C21H35NO4Si2/c1-8-18(22-15-9-10-19(22)23)20(25-27(2,3)4)16-11-13-17(14-15)21

InchiKey:

NEDHARLTVIMVAU-UHFFFAOYSA-N

Formula:

C₂₁H₃₅NO₄Si₂

SMILES:

CCC(C(O[Si](C)(C)C)c1ccc(C(=O)O[Si](C)(C)C)cc1)N1CCCC1=O

Mol. weight [g/mol]:

421.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.12		Crippen Method
logp	4.972		Crippen Method
rinpol	2430.00		NIST Webbook
rinpol	2430.00		NIST Webbook

Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U360395&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/124-635-9/Pyrrolidin-2-one-1-1-4-trimethylsilyloxycarbonylphenyl-butan-1-ol-2-yl-trimethylsilyloxy>

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