

# 1-(4-Trimethylsilyloxycarbonylphenyl)-2-(pyrrolidinyl)butan-1-one

<b>Other names:</b>	4 -methyl-«alpha»-pyrrolidinobutyrophenone-M (carboxy-) TMS
<b>Inchi:</b>	InChI=1S/C18H27NO3Si/c1-5-16(19-12-6-7-13-19)17(20)14-8-10-15(11-9-14)18(21)22-2
<b>InchiKey:</b>	ZUHPCDGGKDXAZ-UHFFFAOYSA-N
<b>Formula:</b>	C18H27NO3Si
<b>SMILES:</b>	CCC(C(=O)c1ccc(C(=O)O[Si](C)(C)C)cc1)N1CCCC1
<b>Mol. weight [g/mol]:</b>	333.50

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.35		Crippen Method
logp	3.735		Crippen Method
rinpol	2220.00		NIST Webbook
rinpol	2220.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U360393&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360393&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>rinpol:</b>	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/124-632-2/1-4-Trimethylsilyloxycarbonylphenyl-2-pyrrolidin-1-yl-butan-1-one.pdf>

Generated by Cheméo on 2024-05-01 02:18:42.954496565 +0000 UTC m=+16819171.875073877.

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