

# Benzoic acid, 4-(1-oxo-2-pyrrolidinohexyl)-, trimethylsilyl ester

Other names:	R,S-4'-methyl-«alpha»-pyrrolidinohexanophenone-M (carboxy), TMS
Inchi:	InChI=1S/C20H31NO3Si/c1-5-6-9-18(21-14-7-8-15-21)19(22)16-10-12-17(13-11-16)20(2
InchiKey:	BMDRZDLTQVVSXHU-UHFFFAOYSA-N
Formula:	C20H31NO3Si
SMILES:	CCCCC(C(=O)c1ccc(C(=O)O[Si](C)(C)C)cc1)N1CCCC1
Mol. weight [g/mol]:	361.55

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.19		Crippen Method
logp	4.516		Crippen Method
rinpol	2390.00		NIST Webbook
rinpol	2390.00		NIST Webbook

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U314306&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U314306&amp;Units=SI</a>

## Legend

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

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