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: BMDRZDLTQVSXHU-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: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U314306&Units=SI

Legend

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