

R,S-4'-methyl-«alpha»-pyrrolidinohexanophenone (carboxy-HO-alkyl)-2TMS

InChI: InChI=1S/C23H39NO4Si2/M-20(27-29(2,3)4)21(24-16-9-10-17-24)22(25)18-12-14-15-13-23
InChIKey: LIXHUYQNESEGUCK-UHFFFAOYSA-N

Formula: C₂₃H₃₉NO₄Si₂
SMILES: CCCC(O[Si](C)(C)C)C(C(=O)c1ccc(C(=O)O[Si](C)(C)C)cc1)N1CCCC1
Mol. weight [g/mol]: 449.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.69		Crippen Method
logp	5.346		Crippen Method
rinpol	2625.00		NIST Webbook
rinpol	2635.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R290794&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

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<https://www.chemeo.com/cid/39-491-4/R-S-4-methyl-alpha-pyrrolidinohexanophenone-M-carboxy-HO-alkyl-2TMS.pdf>

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