

R,S-3',4'-methylenedioxy-«alpha»-pyrrolidinopropiophenone-M-dihydro-TMS

InChI: InChI=1/C17H27NO3Si/c1-13(18-9-5-6-10-18)17(21-22(2,3)4)14-7-8-15-16(11-14)20-19
InChIKey: JJTWCUGCOFJWFN-UHFFFAOYSA-N

Formula: C17H27NO3Si
SMILES: CC(C(O[Si](C)(C)C)c1ccc2c(c1)OCO2)N1CCCC1
Mol. weight [g/mol]: 321.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.01		Crippen Method
logp	3.792		Crippen Method
rinpol	1965.00		NIST Webbook
rinpol	1980.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R290749&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/55-339-5/R-S-3-4-methylenedioxy-alpha-pyrrolidinopropiophenone-M-dihydro-TMS.pdf>

Generated by Cheméo on 2025-12-05 13:54:10.077488722 +0000 UTC m=+4691047.607529376.

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