

Supinine, diTMS

Inchi: InChI=1S/C21H41NO4Si2/c1-16(2)21(26-28(7,8)9,17(3)25-27(4,5)6)20(23)24-15-18-12-11
InchiKey: GHCRMXDRXVNYAI-FBBABVLZSA-N
Formula: C21H41NO4Si2
SMILES: CC(C)C(O[Si](C)(C)C)(C(=O)OCC1=CCN2CCCC12)C(C)O[Si](C)(C)C
Mol. weight [g/mol]: 427.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.06		Crippen Method
logp	4.420		Crippen Method
rinpol	2220.00		NIST Webbook
rinpol	2220.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R252450&Units=SI>

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.chemeo.com/cid/49-691-1/Supinine-diTMS.pdf>

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