

Acetyl ester of echimidine, diTMS

Inchi: InChI=1S/C28H49NO8Si2/c1-13-19(2)25(31)35-23-15-17-29-16-14-22(24(23)29)18-33-2
InchiKey: LJFKXLMDFHMDMQ-TXCNDNEUSA-N
Formula: C28H49NO8Si2
SMILES: CC=C(C)C(=O)OC1CCN2CC=C(COC(=O)C(O[Si](C)(C)C)(C(C)OC(C)=O)C(C)(C)O[Si](C)(C)C
Mol. weight [g/mol]: 583.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.03		Crippen Method
logp	4.594		Crippen Method
rinpol	2870.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R252410&Units=SI>

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.cheméo.com/cid/31-211-2/Acetyl-ester-of-echimidine-diTMS.pdf>

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