

7-tiglyl echinatine, diTMS

Inchi: InChI=1S/C26H47NO6Si2/c1-12-19(4)24(28)31-22-14-16-27-15-13-21(23(22)27)17-30-2
InchiKey: UXBJGYOBHYRFLG-LSPKXPJDSA-N
Formula: C26H47NO6Si2
SMILES: CC=C(C)C(=O)OC1CCN2CC=C(COC(=O)C(O[Si](C)(C)C)(C(C)C)C(C)O[Si](C)(C)C)C12
Mol. weight [g/mol]: 525.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.98		Crippen Method
logp	4.908		Crippen Method
rinpol	2664.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R252396&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/116-046-2/7-tiglyl-echinatine-diTMS.pdf>

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