

Pinobanksin-3-pentanoate, bis-TMS

Inchi: InChI=1S/C26H36O6Si2/c1-8-9-15-22(27)30-26-24(28)23-20(29-25(26)18-13-11-10-12-1
InchiKey: NPNWLLRHTMWYFL-IZZNHLLZSA-N
Formula: C26H36O6Si2
SMILES: CCCCC(=O)OC1C(=O)c2c(cc(O[Si](C)(C)C)cc2O[Si](C)(C)C)OC1c1cccc1
Mol. weight [g/mol]: 500.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.30		Crippen Method
logp	6.532		Crippen Method
rinpol	2838.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R55971&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/40-599-3/Pinobanksin-3-pentanoate-bis-TMS.pdf>

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