Pinobanksin-3-isobutanoate, bis-TMS

Inchi: InChI=1S/C25H34O6Si2/c1-16(2)25(27)29-24-22(26)21-19(28-23(24)17-12-10-9-11-13-1
InchiKey: UVGCRNQPLNICGW-BJKOFHAPSA-N
Formula: C25H34O6Si2
SMILES: CC(C)C(=O)OC1C(=O)c2c(cc(O[Si](C)(C)C)cc2O[Si](C)(C)C)OC1c1ccccc1
Mol. weight [g/mol]: 486.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.64		Crippen Method
logp	5.998		Crippen Method
rinpol	2745.00		NIST Webbook
rinpol	2745.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R55967&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices