Pinobanksin-3-acetate, bis-TMS

Inchi: InChI=1S/C23H30O6Si2/c1-15(24)26-23-21(25)20-18(27-22(23)16-11-9-8-10-12-16)13-1
InchiKey: XZMCDAZMJQSUIN-XZOQPEGZSA-N
Formula: C23H30O6Si2
SMILES: CC(=O)OC1C(=O)c2c(cc(O[Si](C)(C)C)cc2O[Si](C)(C)C)OC1c1ccccc1
Mol. weight [g/mol]: 458.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.05		Crippen Method
logp	5.362		Crippen Method
rinpol	2632.00		NIST Webbook
rinpol	2646.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R55953&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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