

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: XZMCDAZMJQSUIIN-XZOQPEGZSA-N
Formula: C23H30O6Si2
SMILES: CC(=O)OC1C(=O)c2c(cc(O[Si](C)(C)C)cc2O[Si](C)(C)C)OC1c1cccc1
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/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/58-614-6/Pinobanksin-3-acetate-bis-TMS.pdf>

Generated by Cheméo on 2024-04-17 03:49:25.886744565 +0000 UTC m=+15615014.807321877.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.