

Ginkgolide A, TMS ether

Inchi: InChI=1S/C26H40O9Si2/c1-13-18(27)30-16-12-23-15-11-14(22(2,3)4)24(23)17(34-36(5,
InchiKey: LHXSPBWCXALQNT-UHFFFAOYSA-N
Formula: C26H40O9Si2
SMILES: CC1C(=O)OC2CC34C5CC(C(C)(C)C)C36C(OC(=O)C6O[Si](C)(C)C)OC4(C(=O)O5)C21
Mol. weight [g/mol]: 552.76
CAS: 480427-38-1

Physical Properties

Property code	Value	Unit	Source
log10ws	0.02		Crippen Method
logp	3.378		Crippen Method
rinpol	3130.70		NIST Webbook
rinpol	3153.10		NIST Webbook
rinpol	3175.60		NIST Webbook
rinpol	3140.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C480427381&Units=SI>

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/72-150-5/Ginkgolide-A-TMS-ether.pdf>

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