

Ginkgolide C, TMS ether

Inchi: InChI=1S/C29H48O12Si3/c1-14-20(31)35-16-17(39-42(5,6)7)27-22(33)36-18-19(40-43(8)
InchiKey: XARJMBIIZSDZBG-OKUDHBLJSA-N
Formula: C29H48O12Si3
SMILES: CC1C(=O)OC2C(O[Si](C)(C)C)C34OC5OC(=O)C(O)C56C(O)(C(C)(C)C)C(O[Si](C)(C)C)
Mol. weight [g/mol]: 672.94

Physical Properties

Property code	Value	Unit	Source
log10ws	2.52		Crippen Method
logp	2.294		Crippen Method
rinpol	3241.90		NIST Webbook
rinpol	3263.40		NIST Webbook
rinpol	3285.00		NIST Webbook
rinpol	3241.90		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=R203433&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/17-034-5/Ginkgolide-C-TMS-ether.pdf>

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