

Ginkgolide B, TMS ether

Inchi: InChI=1S/C29H48O10Si3/c1-15-21(30)34-19-18(37-40(5,6)7)27-17-14-16(25(2,3)4)26(2
InchiKey: VNOSIJMUIAZKQL-UHFFFAOYSA-N
Formula: C29H48O10Si3
SMILES: CC1C(=O)OC2C(O[Si](C)(C)C)C34C5CC(C(C)(C)C)C36C(OC(=O)C6O[Si](C)(C)C)OC4
Mol. weight [g/mol]: 640.94
CAS: 480427-39-2

Physical Properties

Property code	Value	Unit	Source
log10ws	1.51		Crippen Method
logp	4.208		Crippen Method
rinpol	3235.00		NIST Webbook
rinpol	3259.00		NIST Webbook
rinpol	3190.30		NIST Webbook
rinpol	3190.30		NIST Webbook
rinpol	3211.00		NIST Webbook
rinpol	3211.00		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=C480427392&Units=SI>

Legend

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

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<https://www.cheméo.com/cid/118-091-0/Ginkgolide-B-TMS-ether.pdf>

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