

Ginkgolide J 3TMS

Inchi: InChI=1S/C29H48O10Si3/c1-15-21(30)33-16-14-26-19-17(37-40(5,6)7)18(25(2,3)4)27(28)29
InchiKey: AKKPFRHBJGSCHR-UHFFFAOYSA-N
Formula: C29H48O10Si3
SMILES: CC1C(=O)OC2CC34C5OC(=O)C3(OC3OC(=O)C(O[Si](C)(C)C)C34C(C(C)(C)C)C5O[Si](C)(C)C
Mol. weight [g/mol]: 640.94

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 1.51 | | Crippen Method |
| logp | 4.208 | | Crippen Method |
| rinsol | 3133.70 | | NIST Webbook |
| rinsol | 3133.70 | | 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=U413984&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/117-317-0/Ginkgolide-J-3TMS.pdf>

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