

Laricitrin (5TMS)

Inchi: InChI=1S/C31H52O8Si5/c1-33-25-17-21(18-26(37-42(8,9)10)30(25)38-43(11,12)13)29-3
InchiKey: NCHJXUGHVJJIE-UHFFFAOYSA-N
Formula: C31H52O8Si5
SMILES: COc1cc(-c2oc3cc(O[Si](C)(C)C)cc(O[Si](C)(C)C)c3c(=O)c2O[Si](C)(C)C)cc(O[Si](C)(C)C)C
Mol. weight [g/mol]: 693.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.19		Crippen Method
logp	9.537		Crippen Method
rinpol	3261.60		NIST Webbook
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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=U413961&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/73-594-2/Laricitrin-5TMS.pdf>

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