

Torosachryson, TMS

Inchi: InChI=1S/C25H40O5Si3/c1-25(30-33(9,10)11)15-18-12-17-13-19(27-2)14-21(28-31(3,4))
InchiKey: VZUCNBHFJUCYIC-UHFFFAOYSA-N
Formula: C25H40O5Si3
SMILES: COc1cc(O[Si](C)(C)C)c2c(O[Si](C)(C)C)c3c(cc2c1)CC(C)(O[Si](C)(C)C)CC3=O
Mol. weight [g/mol]: 504.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.69		Crippen Method
logp	7.015		Crippen Method
rinpol	2699.00		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=R158348&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/33-266-0/Torosachryson-TMS.pdf>

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