

THP, TMS

Inchi: InChI=1S/C31H57NO4Si5/c1-37(2,3)32-19-18-25-22-30(35-40(10,11)12)31(36-41(13,14)
InchiKey: IAPRTSNCZDPMNR-UHFFFAOYSA-N
Formula: C31H57NO4Si5
SMILES: C[Si](C)(C)Oc1ccc(CC2c3cc(O[Si](C)(C)C)c(O[Si](C)(C)C)cc3CCN2[Si](C)(C)C)cc1O[Si]
Mol. weight [g/mol]: 648.22

Physical Properties

Property code	Value	Unit	Source
log10ws	1.05		Crippen Method
logp	9.518		Crippen Method
rinpol	2900.00		NIST Webbook
rinpol	2900.00		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=R305094&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/67-498-6/THP-TMS.pdf>

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