

cis-Piceid, 6TMS

Inchi: InChI=1S/C38H70O8Si6/c1-47(2,3)39-28-34-35(44-50(10,11)12)36(45-51(13,14)15)37(4
InchiKey: ZAYPUEYKPPTDBS-VXPUYCOJSA-N
Formula: C38H70O8Si6
SMILES: C[Si](C)(C)OCC1OC(Oc2cc(C=Cc3ccc(O[Si](C)(C)C)cc3)cc(O[Si](C)(C)C)c2)C(O[Si](C)(C)C)C
Mol. weight [g/mol]: 823.47

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 2.08 | | Crippen Method |
| logp | 10.900 | | Crippen Method |
| rinpol | 3308.90 | | NIST Webbook |
| rinpol | 3308.90 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U414023&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/120-127-7/cis-Piceid-6TMS.pdf>

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