

trans-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-FMQUCBEESA-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	3734.90		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U414022&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/120-128-6/trans-Piceid-6TMS.pdf>

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