

Theandrose: aD-Gclp(1->6)-aDGlc(1->2)-DFru, oxime-TMS

Inchi: InChI=1S/C50H118O16Si11/c1-67(2,3)53-35-38-40(58-69(7,8)9)42(60-71(13,14)15)43(6
InchiKey: OEPGHTDGQMCMX-FJJNRPAVSA-N
Formula: C50H118O16Si11
SMILES: C[Si](C)(C)OCC1OC(OCC2OC(OCC3(O[Si](C)(C)C)OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C3
Mol. weight [g/mol]: 1284.40

Physical Properties

Property code	Value	Unit	Source
log10ws	12.06		Crippen Method
logp	12.837		Crippen Method
rinpol	3320.00		NIST Webbook
rinpol	3320.00		NIST Webbook

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=R588942&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/113-716-1/Theandrose-aD-Gclp-1-6-aDGlc-1-2-DFru-oxime-TMS.pdf>

Generated by Cheméo on 2024-04-28 20:17:23.15936165 +0000 UTC m=+16624692.079938962.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.