

Cellotriose: bD-Glcp(1->4)-bDGlcp(1->4)-DGlc, oxime-TMS, isomer # 1

Inchi: InChI=1S/C54H129NO16Si12/c1-72(2,3)56-38-42-45(61-54-52(70-82(31,32)33)50(68-80)
InchiKey: HSCPJKJOFDBMNBE-ZOBWJYGWSA-N
Formula: C54H129NO16Si12
SMILES: C[Si](C)(C)OCC(O[Si](C)(C)C)C(OC1OC(CO[Si](C)(C)C)C(OC2OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C)C1O
Mol. weight [g/mol]: 1385.63

Physical Properties

Property code	Value	Unit	Source
log10ws	13.07		Crippen Method
logp	14.359		Crippen Method
rinpol	3415.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R588799&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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<https://www.cheméo.com/cid/70-807-8/Cellotriose-bD-Glcp-1-4-bDGlcp-1-4-DGlc-oxime-TMS-isomer-1.pdf>

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