

6'-Glucosyl-gentobiose: aD-Glcp(1->6)-bDGlc(1->6)-DGlc, oxime-TMS, Isomer # 2

InChI: InChI=1S/C54H129NO16Si12/c1-72(2,3)58-40-43-47(65-77(16,17)18)50(68-80(25,26)27-28)19-21-22-23-24-25-26-27-28-29-30-31-32-33-34-35-36-37-38-39-41-42-44-45-46-48-49-51-52-53-54/s1-12/t1-12

InChIKey: JTWAMTXXTTJEATF-OVLOVKAPSA-N

Formula: C54H129NO16Si12

SMILES: C[Si](C)(C)OCC1OC(OCC2OC(OCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(C=

Mol. weight [g/mol]: 1385.63

Physical Properties

Property code	Value	Unit	Source
log10ws	13.07		Crippen Method
logp	14.359		Crippen Method
rinpol	3594.00		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=R588784&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/67-238-4/6-Glucosyl-gentobiose-aD-Glcp-1-6-bDGlc-1-6-DGlc-oxime-TMS-isomer-2.p>

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