

Nigerotriose:
aD-Glcp(1->3)-aDGlc(1->3)-DGlc, oxime-TMS,
Isomer # 2

InChI: InChI=1S/C54H129NO16Si12/c1-72(2,3)56-38-42-46(65-77(16,17)18)49(62-54-52(70-82
InChIKey: KBXQQCBUZUFDIW-QLTLVVBXSA-N

Formula: C54H129NO16Si12

SMILES: C[Si](C)(C)OCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(OC1OC(CO[Si](C)(C)C)C(O[Si](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
rmpol	3488.00		NIST Webbook
rmpol	3488.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R588922&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rmpol: Non-polar retention indices

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<https://www.cheméo.com/cid/125-141-6/Nigerotriose-aD-Glcp-1-3-aDGlc-1-3-DGlc-oxime-TMS-isomer-2.pdf>

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