

Isomaltotriose:
aD-Glcp(1->6)-aDGlcp(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
InChIKey: JTWAMTXXTTJEATF-CPBGQDAFSA-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	3647.00		NIST Webbook
rinpol	3711.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R588660&Units=SI>

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

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

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/32-411-9/Isomaltotriose-aD-Glcp-1-6-aDGlcp-1-6-DGlc-oxime-TMS-isomer-2.pdf>

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