

3'-Glucosyl-isomaltose: aD-Glcp(1->3)-aDGlc(1->6)-DGlc, oxime-TMS, Isomer # 1

InChI: InChI=1S/C54H129NO16Si12/c1-72(2,3)57-39-42-46(65-77(16,17)18)49(61-54-52(70-82
InChIKey: BELXNDVTTTPSCNY-OVLOVKAPSA-N
Formula: C54H129NO16Si12
SMILES: C[Si](C)(C)OCC1OC(OCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(C=NO[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
rinpol	3558.00		NIST Webbook
rinpol	3558.00		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=R588695&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/115-939-2/3-Glucosyl-isomaltose-aD-Glcp-1-3-aDGlc-1-6-DGlc-oxime-TMS-isomer-1>

Generated by Cheméo on 2024-05-06 16:51:22.077726487 +0000 UTC m=+17303530.998303809.

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