

Galactotriose:
aD-Galp(1->3)-bDGalp(1->4)-DGal, oxime-TMS,
Isomer # 1

InChI: InChI=1S/C54H129NO16Si12/c1-72(2,3)56-38-42-47(66-78(19,20)21)49(62-54-52(70-82
InChIKey: AMBHMSTZMXJKJV-SCQJAHKUSA-N

Formula: C54H129NO16Si12

SMILES: C[Si](C)(C)OCC(O[Si](C)(C)C)C(OC1OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C(OC2OC(CO[Si](C)(C)C)C)C1O2

Mol. weight [g/mol]: 1385.63

Physical Properties

Property code	Value	Unit	Source
log10ws	13.07		Crippen Method
logp	14.359		Crippen Method
rinpol	3425.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R588813&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/70-791-6/Galactotriose-aD-Galp-1-3-bDGalp-1-4-DGal-oxime-TMS-isomer-1.pdf>

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