

Inulotriose: bD-Fruf(2->1)-bDFruf(2->1)-DFru, oxime-TMS, isomer # 1

Inchi: InChI=1S/C48H114O16Si11/c1-65(2,3)51-36-47(41(59-70(16,17)18)38(56-67(7,8)9)44(5
InchiKey: BTVJTZCZVGMZJI-VMMWBGMCSA-N
Formula: C48H114O16Si11
SMILES: C[Si](C)(C)OCC1(OCC2(OCC3(O[Si](C)(C)C)OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C3O[Si](C)(C)C)OCC1
Mol. weight [g/mol]: 1256.35

Physical Properties

Property code	Value	Unit	Source
log10ws	12.13		Crippen Method
logp	12.755		Crippen Method
rinpol	3284.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R588848&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/46-866-0/Inulotriose-bD-Fruf-2-1-bDFruf-2-1-DFru-oxime-TMS-isomer-1.pdf>

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