

CELLOTRIOSE (11TMS)

Inchi: InChI=1S/C51H120O16Si11/c1-68(2,3)52-34-37-40(58-50-47(65-76(25,26)27)45(63-74(

InchiKey: HRWJJBNTMIKSP-VXNDBNCOSA-N

Formula: C51H120O16Si11

SMILES: C[Si](C)(C)OCC1OC(OC2C(CO[Si](C)(C)C)OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C2O[Si](C)(

Mol. weight [g/mol]: 1298.43

Physical Properties

Property code	Value	Unit	Source
log10ws	12.03		Crippen Method
logp	12.878		Crippen Method
rinpol	3530.50		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R414490&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/67-518-3/CELLOTRIOSE-11TMS.pdf>

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