

Melezitose, 11TMS

Inchi: InChI=1S/C51H120O16Si11/c1-68(2,3)52-34-38-41(61-72(13,14)15)44(64-75(22,23)24)4
InchiKey: XGLGJEYXDSXZPD-KQJPMKKJSA-N
Formula: C51H120O16Si11
SMILES: C[Si](C)(C)OCC1OC(OC2C(O[Si](C)(C)C)C(CO[Si](C)(C)C)OC2(CO[Si](C)(C)C)OC2OC
Mol. weight [g/mol]: 1298.43

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 12.14 | | Crippen Method |
| logp | 12.880 | | Crippen Method |
| rinsol | 3476.00 | | NIST Webbook |
| rinsol | 3476.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R605973&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinsol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/119-557-2/Melezitose-11TMS.pdf>

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