

Sucrose, TMS # 1

Inchi: InChI=1S/C36H86O11Si8/c1-48(2,3)37-25-28-30(43-51(10,11)12)32(45-53(16,17)18)33(44)19-27-29-31(42)41-47-46-34-35-36
InchiKey: JDAONBLATRVCRV-PMPIGOBISA-N
Formula: C36H86O11Si8
SMILES: C[Si](C)(C)OCC1OC(OC2(CO[Si](C)(C)C)OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C2O[Si](C)(C)C
Mol. weight [g/mol]: 919.75

Physical Properties

Property code	Value	Unit	Source
log10ws	8.95		Crippen Method
logp	9.478		Crippen Method
rinpol	3035.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R631739&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/71-734-8/Sucrose-TMS-1.pdf>

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