

«alpha»-Neolactose, TMS

Inchi: InChI=1S/C36H86O11Si8/c1-48(2,3)37-25-27-30(43-51(10,11)12)32(45-53(16,17)18)34(19,20)21-22-23-24-26-28-29(31-35)33-36
InchiKey: BKRCJVHGUNBEML-VJTRPLOFSA-N
Formula: C36H86O11Si8
SMILES: C[Si](C)(C)OCC1OC(O[Si](C)(C)C)C(OC2OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1
Mol. weight [g/mol]: 919.75

Physical Properties

Property code	Value	Unit	Source
log10ws	8.84		Crippen Method
logp	9.476		Crippen Method
rinsol	2671.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R67926&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/27-479-1/alpha-Neolactose-TMS.pdf>

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