

2-deoxyglucitol, TMS

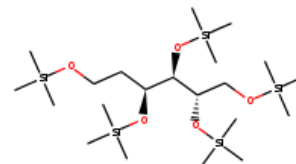
InChI: InChI=1S/C21H54O5Si5/c1-27(2,3)22-17-16-19(24-29(7,8)9)21(26-31(13,14)15)20(25-30(10,11)12)18-23-28(4,5)6/h19-21H,16-18H2,1-15H3

InChI Key: ULCPMKYKEVLMSQ-UHFFFAOYSA-N

Formula: C₂₁H₅₄O₅Si₅

SMILES: C[Si](C)(C)OCCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](C)(C)C

Molecular Weight: 527.08



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	6.740		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H54O5Si5/c1-27\(2,3\)22-17-16-19\(24-29\(7,8\)9\)21\(26-31\(13,14\)15\)20\(25-30\(10,11\)12\)18-23-28\(4,5\)6/h19-21H,16-18H2,1-15H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H54O5Si5/c1-27(2,3)22-17-16-19(24-29(7,8)9)21(26-31(13,14)15)20(25-30(10,11)12)18-23-28(4,5)6/h19-21H,16-18H2,1-15H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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