

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)5-4-3-2-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29-30-31-32-33-34-35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100
InchiKey: 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
Mol. weight [g/mol]: 527.08

Physical Properties

Property code	Value	Unit	Source
log10ws	5.36		Crippen Method
logp	6.740		Crippen Method
rinpol	1859.70		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R488832&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/40-484-0/2-deoxyglucitol-TMS.pdf>

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