

3-Deoxy-lyxo-hexaric acid, TMS

Inchi: InChI=1S/C21H50O7Si5/c1-29(2,3)24-17(19(26-31(7,8)9)21(23)28-33(13,14)15)16-18(20)12-22
InchiKey: ZJKJLJLIOZASHHC-GBESFXJTSA-N
Formula: C₂₁H₅₀O₇Si₅
SMILES: C[Si](C)(C)OC(=O)C(CC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 555.04

Physical Properties

Property code	Value	Unit	Source
log10ws	5.81		Crippen Method
logp	5.793		Crippen Method
rinpol	1956.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R101298&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/11-974-8/3-Deoxy-lyxo-hexaric-acid-TMS.pdf>

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