

Glucose, MO-TMS

Inchi: InChI=1S/C22H55NO6Si5/c1-24-23-17-19(26-31(5,6)7)21(28-33(11,12)13)22(29-34(14,15)16)30(17,18)O/Si(C)(C)C(Si(C)(C)C(Si(C)(C)C(Si(C)(C)C(Si(C)(C)C(CO[Si](C)(C)C)O[Si](C)(C)C)O[Si](C)(C)C)O[Si](C)(C)C)O[Si](C)(C)C

InchiKey: LLVFXKDPAPSCJ-XWIKXRDFSAN

Formula: C22H55NO6Si5

SMILES: CON=CC(O[Si](C)(C)C)C(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]: 570.10

Physical Properties

Property code	Value	Unit	Source
log10ws	5.59		Crippen Method
logp	6.350		Crippen Method
rinpol	1886.00		NIST Webbook
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Sources

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R604158&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/114-162-5/Glucose-MO-TMS.pdf>

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