

2-Deoxyglucose, MO-TMS

Inchi: InChI=1S/C21H53NO5Si5/c1-28(2,3)23-18-20(25-30(7,8)9)21(26-31(10,11)12)19(24-29)
InchiKey: VXOJCDPQIHSVGI-WZHCGWADSA-N
Formula: C21H53NO5Si5
SMILES: C[Si](C)(C)OCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(CC=NO[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 540.08

Physical Properties

Property code	Value	Unit	Source
log10ws	5.21		Crippen Method
logp	6.726		Crippen Method
rinpol	1825.00		NIST Webbook
rinpol	1830.00		NIST Webbook

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=R529923&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/21-553-4/2-Deoxyglucose-MO-TMS.pdf>

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