

[2H]Glucosamine, TMS

Inchi: InChI=1S/C21H53NO5Si5/c1-28(2,3)22-18-20(26-31(10,11)12)19(25-30(7,8)9)17(16-23-
InchiKey: AEFMNTFHQDMWON-PSTSCRTLSA-N
Formula: C21H53NO5Si5
SMILES: C[Si](C)(C)NC1C(O[Si](C)(C)C)OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 540.08

Physical Properties

Property code	Value	Unit	Source
log10ws	5.56		Crippen Method
logp	5.648		Crippen Method
rinsol	1990.00		NIST Webbook
rinsol	1990.00		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=R176391&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinsol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/56-982-0/2H-Glucosamine-TMS.pdf>

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