«beta»-N-Acetyl-D-glucosamine, TMS

Inchi: InChI=1S/C19H45NO6Si4/c1-14(21)20-15-16(23-27(2,3)4)17(24-28(5,6)7)19(26-30(11,1
InchiKey: HUXJBHUJRMWUPT-QTMHVTGLSA-N
Formula: C19H45NO6Si4
SMILES: CC(=O)NC1C(O[Si](C)(C)C)OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 495.91

Physical Properties

Property code	Value	Unit	Source
logp	4.317		Crippen Method
rinpol	2144.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R441100&Units=SI

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:
https://www.chemeo.com/cid/27-709-5/beta-N-Acetyl-D-glucosamine-TMS.pdf
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