

N-Acetyl-D-glucosamine, tetrakis(trimethylsilyl) ether, benzyloxime

(isomer 1)

InChI: InChI=1S/C27H54N2O6Si4/c1-22(30)29-24(19-28-31-20-23-17-15-14-16-18-23)26(34-38)27(39-40)13-12-11-10-9-8-7-6-5-4-3-2-1
InChIKey: YEUBXDOSNQDXNS-UHFFFAOYSA-N

Formula: C27H54N2O6Si4

SMILES: CC(=O)NC(C=NOCc1ccccc1)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]: 615.07

Physical Properties

Property code	Value	Unit	Source
log10ws	2.07		Crippen Method
logp	6.206		Crippen Method
rinpol	2594.20		NIST Webbook
rinpol	2594.20		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=U380347&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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