

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

InChI:
(syn)

InChI=1S/C21H50N2O6Si4/c1-17(24)23-18(15-22-25-2)20(28-32(9,10)11)21(29-33(12,13)14)

InChI Key:

CKZSFVYLUTZEAC-UHFFFAOYSA-N

Formula:

C₂₁H₅₀N₂O₆Si₄

SMILES:

CON=CC(NC(C)=O)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]:

538.97

Physical Properties

Property code	Value	Unit	Source
log10ws	4.18		Crippen Method
logp	4.635		Crippen Method
rinsol	2067.50		NIST Webbook
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Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U380193&Units=SI>

Crippen Method:

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

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/19-012-7/N-Acetyl-D-glucosamine-tetrakis-trimethylsilyl-ether-methyloxime-syn.pdf>

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