N-Acetyl-D-galactosaminitol, pentakis(trimethylsilyl) ether

Inchi: InChI=1S/C23H57NO6Si5/c1-19(25)24-20(17-26-31(2,3)4)22(29-34(11,12)13)23(30-35(1

InchiKey: RAXPVCSDMAMRLJ-UHFFFAOYSA-N

Formula: C23H57NO6Si5

SMILES: CC(=O)NC(CO[Si](C)(C)C)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]: 584.13

Physical Properties

Property code	Value	Unit	Source
log10ws	5.45		Crippen Method
logp	5.854		Crippen Method
rinpol	2070.70		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U380258&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices