Pseudo uridine penta-tms

Other names: «beta»-Pseudouridine, TMS
Inchi: InChI=1S/C24H52N2O6Si5/c1-33(2,3)27-17-19-21(29-34(4,5)6)22(30-35(7,8)9)20(28-19
InchiKey: XHLZQKAETJELAB-UHFFFAOYSA-N
Formula: C24H52N2O6Si5
SMILES: C[Si](C)(C)OCC1OC(c2cnc(O[Si](C)(C)C)nc2O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C
Mol. weight [g/mol]: 605.11
CAS: 53294-25-0

Physical Properties

Property code	Value	Unit	Source
log10ws	3.96		Crippen Method
logp	6.636		Crippen Method
rinpol	2375.00		NIST Webbook
rinpol	2375.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C53294250&Units=SI

Legend

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