D-(-)-Tagatose, pentakis(trimethylsilyl) ether

Inchi: InChI=1S/C21H52O6Si5/c1-28(2,3)23-16-18(22)20(26-31(10,11)12)21(27-32(13,14)15)1
InchiKey: LDUCAYFXHYLHLP-UHFFFAOYSA-N
Formula: C21H52O6Si5
SMILES: C[Si](C)(C)OCC(=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]: 541.06

Physical Properties

Property code	Value	Unit	Source
log10ws	6.08		Crippen Method
logp	5.919		Crippen Method
rinpol	1878.30		NIST Webbook
rinpol	1878.30		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U380124&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