D(-)-Tagatose, aldol, TMS

Inchi: InChI=1S/C21H52O6Si5/c1-28(2,3)23-17-19(25-30(7,8)9)21(27-32(13,14)15)20(26-31(10
InchiKey: PPTMWEDTYQRQBC-VKEMMKHGSA-N
Formula: C21H52O6Si5
SMILES: C[Si](C)(C)OCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(C=O)O[Si](C)(C)C
Mol. weight [g/mol]: 541.06

Physical Properties

Property code	Value	Unit	Source
log10ws	5.97		Crippen Method
logp	5.917		Crippen Method
rinpol	1934.00		NIST Webbook
rinpol	1934.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R441299&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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