2-C-Methylarabinonic acid, pentakis-TMS

Inchi: InChI=1S/C21H52O6Si5/c1-21(27-32(14,15)16,20(22)26-31(11,12)13)19(25-30(8,9)10)1
InchiKey: SOYWKUNHUVGLPR-GZNCHQMQSA-N
Formula: C21H52O6Si5
SMILES: CC(O[Si](C)(C)C)(C(=O)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	5.59		Crippen Method
logp	6.266		Crippen Method
rinpol	1876.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R100839&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