Xylaric acid, TMS

Inchi: InChI=1S/C20H48O7Si5/c1-28(2,3)23-16(17(24-29(4,5)6)19(21)26-31(10,11)12)18(25-30
InchiKey: QGJKSEWJPVGCIU-NNZMDNLPSA-N
Formula: C20H48O7Si5
SMILES: C[Si](C)(C)OC(=O)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 541.02

Physical Properties

Property code	Value	Unit	Source
log10ws	6.23		Crippen Method
logp	5.403		Crippen Method
rinpol	1872.00		NIST Webbook
rinpol	1872.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R101996&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