

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)5-7-8-9-13-14-15-22-27-28-29-30-31-32-33-34-35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100
InchiKey: QGJKSEWJPVGC IU-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
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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

Latest version available from:

<https://www.chemeo.com/cid/51-314-6/Xylaric-acid-TMS.pdf>

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