

«beta»-D-Xylulose, TMS

Inchi: InChI=1S/C17H42O5Si4/c1-23(2,3)19-14-17(22-26(10,11)12)16(21-25(7,8)9)15(13-18-17)
InchiKey: APQKDYOCVZXJBM-YESZJQIVSA-N
Formula: C17H42O5Si4
SMILES: C[Si](C)(C)OCC1(O[Si](C)(C)C)OCC(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 438.85

Physical Properties

Property code	Value	Unit	Source
log10ws	4.70		Crippen Method
logp	4.856		Crippen Method
rinpol	1605.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R441051&Units=SI>

Legend

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

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<https://www.cheméo.com/cid/54-288-3/beta-D-Xylulose-TMS.pdf>

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