D-Xylulose, ketol, TMS

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

Physical Properties

Property code	Value	Unit	Source
log10ws	5.00		Crippen Method
logp	4.699		Crippen Method
rinpol	1718.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R441388&Units=SI

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/25-947-3/D-Xylulose-ketol-TMS.pdf

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