

«beta»-Fructopyranose, TMS

Other names:	«beta»-D(-)-Fructose (Levulose), pyranose, TMS
Inchi:	InChI=1S/C21H52O6Si5/c1-28(2,3)23-17-21(27-32(13,14)15)20(26-31(10,11)12)19(25-3
InchiKey:	PJXWXHJDJODISP-ILRWHQKPSA-N
Formula:	C21H52O6Si5
SMILES:	C[Si](C)(C)OCC1(O[Si](C)(C)C)OCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]:	541.06

Physical Properties

Property code	Value	Unit	Source
log10ws	5.77		Crippen Method
logp	6.076		Crippen Method
rinpol	1930.00		NIST Webbook
ripol	1685.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R389601&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/42-300-1/beta-Fructopyranose-TMS.pdf>

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