

Fructose, MO-TMS, I

Inchi: InChI=1S/C22H55NO6Si5/c1-24-23-19(17-25-30(2,3)4)21(28-33(11,12)13)22(29-34(14,15)16)20(18,27)10(26)5
InchiKey: ACDMQGXCXUQPRR-YPAWHYETSA-N
Formula: C22H55NO6Si5
SMILES: CON=C(CO[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 570.10

Physical Properties

Property code	Value	Unit	Source
log10ws	5.70		Crippen Method
logp	6.352		Crippen Method
rinpol	1925.00		NIST Webbook
rinpol	1935.00		NIST Webbook
rinpol	1925.00		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=R529958&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/70-075-1/Fructose-MO-TMS-I.pdf>

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