

Fructose-6-phosphate, MO-TMS

Inchi: InChI=1S/C25H64NO9PSi6/c1-28-26-22(20-30-37(2,3)4)24(32-39(8,9)10)25(33-40(11,12)31)6
InchiKey: PYLXLHQAZZMFRY-UYKXPLQNSA-N
Formula: C25H64NO9PSi6
SMILES: CON=C(CO[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(COP(=O)(O[Si](C)(C)C)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 722.26

Physical Properties

Property code	Value	Unit	Source
log10ws	4.95		Crippen Method
logp	8.328		Crippen Method
rinpol	2292.00		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=R604123&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/124-300-0/Fructose-6-phosphate-MO-TMS.pdf>

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