

myo-Inositol phosphate, heptakis-TMS

Inchi: InChI=1S/C27H69O9PSi7/c1-38(2,3)30-23-22(29-37(28,35-43(16,17)18)36-44(19,20)21)
InchiKey: WOZUKLPEHGPIJE-CNLNYYNNXSA-N
Formula: C27H69O9PSi7
SMILES: C[Si](C)(C)OC1C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(OP(=O)(O[Si](C)(C)C)O[Si](C)(C)C)C(C)C
Mol. weight [g/mol]: 765.40

Physical Properties

Property code	Value	Unit	Source
log10ws	5.99		Crippen Method
logp	9.297		Crippen Method
rinpol	2479.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R573678&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/61-136-3/myo-Inositol-phosphate-heptakis-TMS.pdf>

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