

xanthosine-5'-monophosphate, TMS

Inchi: InChI=1S/C28H61N4O9PSi6/c1-43(2,3)36-23-21(19-34-42(33,40-47(13,14)15)41-48(16,
InchiKey: JGBBDPOOSQSHSG-UHFFFAOYSA-N
Formula: C28H61N4O9PSi6
SMILES: C[Si](C)(C)Oc1nc(O[Si](C)(C)C)c2ncn(C3OC(COP(=O)(O[Si](C)(C)C)O[Si](C)(C)C)C(O[Si](C)(C)C)C
Mol. weight [g/mol]: 797.29

Physical Properties

Property code	Value	Unit	Source
log10ws	2.19		Crippen Method
logp	8.419		Crippen Method
rinpol	3134.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R207257&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/53-609-7/xanthosine-5-monophosphate-TMS.pdf>

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