inosine-5'-monophosphate, TMS

Inchi:	InChI=1S/C25H53N4O8PSi5/c1-39(2,3)33-21-19(16-31-38(30,36-42(10,11)12)37-43(13,
InchiKey:	HHRWZMFMIFMUOO-UHFFFAOYSA-N
Formula:	C25H53N4O8PSi5
SMILES:	C[Si](C)(C)Oc1ncnc2c1ncn2C1OC(COP(=O)(O[Si](C)(C)C)O[Si](C)(C)C)C(O[Si](C)(C)C
Mol. weight [g/mol]:	709.11

Physical Properties

Property code	Value	Unit	Source
log10ws	1.20		Crippen Method
logp	7.205		Crippen Method
rinpol	3040.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R207153&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/72-254-0/inosine-5-monophosphate-TMS.pdf

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