

# 9H-Purine, 9-[2-deoxy-3-O-(trimethylsilyl)-«beta»-D-erythro-p 5-[bis(trimethylsilyl) phosphate]

<b>Aliases:</b>	Deoxyguanosine-5'-monophosphate, (5-TMS) deoxyguanosine-5'-monophosphate, TMS
<b>Inchi:</b>	InChI=1S/C25H54N5O7PSi5/c1-39(2,3)29-25-27-23-22(24(28-25)35-41(7,8)9)26-18-30(
<b>InchiKey:</b>	XZVVKKUHQCSABN-UHFFFAOYSA-N
<b>Formula:</b>	C25H54N5O7PSi5
<b>SMILES:</b>	C[Si](C)(C)Nc1nc(O[Si](C)(C)C)c2ncn(C3CC(O[Si](C)(C)C)C(COP(=O)(O[Si](C)(C)C)O[S
<b>Mol. weight [g/mol]:</b>	708.13
<b>CAS:</b>	32645-71-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.81		Crippen Method
logp	7.622		Crippen Method
rinpol	3224.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C32645719&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C32645719&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>rinpol:</b>	Non-polar retention indices

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