

1H-Purine-2,6,8(3H)-trione, 4,9-dihydro-1,3,4,9-tetrakis(trimethylsilyl)-

Other names:	Uric acid, tetra-TMS
Inchi:	InChI=1S/C17H36N4O3Si4/c1-25(2,3)17-13(18-15(23)20(17)27(7,8)9)14(22)19(26(4,5)6
InchiKey:	ZLRODCMJWNXARV-UHFFFAOYSA-N
Formula:	C17H36N4O3Si4
SMILES:	C[Si](C)(C)N1C(=O)C2=NC(=O)N([Si](C)(C)C)C2([Si](C)(C)C)N([Si](C)(C)C)C1=O
Mol. weight [g/mol]:	456.83
CAS:	55530-45-5

Physical Properties

Property code	Value	Unit	Source
log10ws	4.80		Crippen Method
logp	4.206		Crippen Method
rinpol	2127.00		NIST Webbook
rinpol	2110.00		NIST Webbook
rinpol	2141.00		NIST Webbook
rinpol	2127.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55530455&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/118-450-1/1H-Purine-2-6-8-3H-trione-4-9-dihydro-1-3-4-9-tetrakis-trimethylsilyl.pdf>

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