

1-Methylhypoxanthine riboside, TMS

Inchi: InChI=1S/C20H38N4O5Si3/c1-23-12-22-18(25)15-19(23)24(13-21-15)20-17(29-32(8,9)1
InchiKey: BDBLFYSIFUZVGW-FIALEDGQSA-N
Formula: C20H38N4O5Si3
SMILES: Cn1cnc(=O)c2ncn(C3OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C3O[Si](C)(C)C)c21
Mol. weight [g/mol]: 498.80

Physical Properties

Property code	Value	Unit	Source
log10ws	6.86e-03		Crippen Method
logp	3.319		Crippen Method
rinpol	2980.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R93515&Units=SI>

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/62-654-7/1-Methylhypoxanthine-riboside-TMS.pdf>

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