

adenosine-2'-monophosphate, TMS

Inchi: InChI=1S/C25H54N5O7PSi5/c1-39(2,3)29-23-20-24(27-17-26-23)30(18-28-20)25-22(34-33)21-26
InchiKey: CMYBPUAOETZXMJ-UHFFFAOYSA-N
Formula: C₂₅H₅₄N₅O₇PSi₅
SMILES: C[Si](C)(C)Nc1ncnc2c1ncn2C1OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C1OP(=O)(O[Si](C)(C)C)C1
Mol. weight [g/mol]: 708.13

Physical Properties

Property code	Value	Unit	Source
log10ws	1.31		Crippen Method
logp	7.238		Crippen Method
rinpol	3006.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R207019&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/119-084-7/adenosine-2-monophosphate-TMS.pdf>

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