

5,6-Dimethyladenine, TMS

Inchi: InChI=1S/C10H17N5Si/c1-7-13-9-8(15(7)2)10(12-6-11-9)14-16(3,4)5/h6H,1-5H3,(H,11,12)
InchiKey: CLKVPXOHPZUVKI-UHFFFAOYSA-N
Formula: C₁₀H₁₇N₅Si
SMILES: Cc1nc2ncnc(N[Si](C)(C)C)c2n1C
Mol. weight [g/mol]: 235.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.23		Crippen Method
logp	1.919		Crippen Method
rinpol	1786.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R93793&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/29-575-2/5-6-Dimethyladenine-TMS.pdf>

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