

6-Methylpurine, TMS

Inchi: InChI=1S/C9H14N4Si/c1-7-12-9-8(5-10-6-11-9)13(7)14(2,3)4/h5-6H,1-4H3
InchiKey: YCZBAWWSDXEAAQ-UHFFFAOYSA-N
Formula: C9H14N4Si
SMILES: Cc1nc2ncncc2n1[Si](C)(C)C
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.39		Crippen Method
logp	1.818		Crippen Method
rinpol	1518.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R93967&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/60-670-1/6-Methylpurine-TMS.pdf>

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