

Purine, 6-hydroxy, TMS

Inchi: InChI=1S/C8H12N4OSi/c1-14(2,3)13-8-6-7(10-4-9-6)11-5-12-8/h4-5H,1-3H3,(H,9,10,11,
InchiKey: WDSAHFJXJSONVER-UHFFFAOYSA-N
Formula: C8H12N4OSi
SMILES: C[Si](C)(C)Oc1ncnc2nc[nH]c12
Mol. weight [g/mol]: 208.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.80		Crippen Method
logp	1.085		Crippen Method
rinpol	1796.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R386642&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/23-263-4/Purine-6-hydroxy-TMS.pdf>

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