6-Azauracil, TMS

Inchi: InChI=1S/C9H19N3O2Si2/c1-15(2,3)13-8-7-10-12-9(11-8)14-16(4,5)6/h7H,1-6H3
InchiKey: MNMOUFWORYTNCL-UHFFFAOYSA-N
Formula: C9H19N3O2Si2
SMILES: C[Si](C)(C)Oc1cnnc(O[Si](C)(C)C)n1
Mol. weight [g/mol]: 257.44

Physical Properties

Property code	Value	Unit	Source
log10ws	1.22		Crippen Method
logp	2.299		Crippen Method
rinpol	1449.90		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1449.90		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R5988&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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