Purine, 6-(3-methyl-2-butenyl)amino, TMS

Inchi: InChI=1S/C13H21N5Si/c1-10(2)6-7-18(19(3,4)5)13-11-12(15-8-14-11)16-9-17-13/h6,8-9
InchiKey: PRNLBRLDGJUCOT-UHFFFAOYSA-N
Formula: C13H21N5Si
SMILES: CC(C)=CCN(c1ncnc2[nH]cnc12)[Si](C)(C)C
Mol. weight [g/mol]: 275.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.12		Crippen Method
logp	2.479		Crippen Method
rinpol	2125.00		NIST Webbook
rinpol	2125.00		NIST Webbook

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=R386533&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices