

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: PRNLBRLDGGJUCOT-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/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/83-229-6/Purine-6-3-methyl-2-butenyl-amino-TMS.pdf>

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