9H-Purin-6-amine, N,N-dimethyl-9-(trimethylsilyl)-

Other names: Adenine, N,N-dimethyl-9-(trimethylsilyl)-
Dimethylaminopurine, N-trimethylsilyl-
N,N-Dimethyl-9-(trimethylsilyl)-9H-purin-6-amine
6-Dimethyladenine, TMS
6-(Dimethylamino)purine, tms derivative

Inchi: InChI=1S/C10H17N5Si/c1-14(2)9-8-10(12-6-11-9)15(7-13-8)16(3,4)5/h6-7H,1-5H3

InchiKey: XILWLVGCTPVKKT-UHFFFAOYSA-N

Formula: C10H17N5Si

SMILES: CN(C)c1ncnc2c1ncn2[Si](C)(C)C

Mol. weight [g/mol]: 235.36

CAS: 32865-76-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.82		Crippen Method
logp	1.575		Crippen Method
rinpol	1850.40		NIST Webbook
rinpol	1850.40		NIST Webbook
rinpol	1795.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C32865762&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