

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

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