3H-PURIN-6-AMINE, 3-METHYL-

Other names:	3H-Purin-6-amine, 3-methyl-
	Adenine, 3-methyl-
	3-Methyladenine
	3-methyl-3H-adenine
Inchi:	InChI=1S/C6H7N5/c1-11-3-10-5(7)4-6(11)9-2-8-4/h2-3H,7H2,1H3
InchiKey:	FSASIHFSFGAIJM-UHFFFAOYSA-N
Formula:	C6H7N5
SMILES:	Cn1cnc(N)c2ncnc1-2
Mol. weight [g/mol]:	149.16

Physical Properties

Property code	Value	Unit	Source
ie	8.52	eV	Cheméo Relay (1.0)
logp	-0.103		Crippen Method
mcvol	106.380	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5142234&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Latest version available from:

https://www.chemeo.com/cid/15-296-7/3H-PURIN-6-AMINE-3-METHYL.pdf

Generated by Cheméo on 2026-07-27 06:25:45.870993695 +0000 UTC m=+59171.905108942.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.