1-METHYLADENINE

Other names:	1-methyladenine
	1H-Purin-6-amine, 1-methyl-
	6H-Purin-6-imine, 1,9-dihydro-1-methyl-
	Adenine, 1-methyl-
Inchi:	InChI=1S/C6H7N5/c1-11-3-10-6-4(5(11)7)8-2-9-6/h2-3H,7H2,1H3
InchiKey:	HPZMWTNATZPBIH-UHFFFAOYSA-N
Formula:	C6H7N5
SMILES:	Cn1cnc2ncnc-2c1N
Mol. weight [g/mol]:	149.16

Physical Properties

Property code	Value	Unit	Source
ie	8.48	eV	Cheméo Relay (1.0)
logp	-0.103		Crippen Method
mcvol	106.380	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5142223&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

Cheméo Relay (1.0):

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume