Adenine

Other names:	1,6-Dihydro-6-iminopurine
	1H-Purin-6-amine
	1H-Purine, 6-amino-
	1H-Purine-6-amine
	3,6-Dihydro-6-iminopurine
	6-Amino-1H-purine
	6-Amino-3H-purine
	6-Amino-7H-purine
	6-Amino-9H-purine
	6-Aminopurine
	9H-Purin-6-yl-amine
	9H-Purine, 1,6-dihydro-6-imino-
	9H-Purine-6-amine
	ADE
	Adenin
	Adeninimine
	Leuco-4
	NSC 14666
	Purine, 6-amino-
	USAF CB-18
	Vitamin B4
Inchi:	InChI=1S/C5H5N5/c6-4-3-5(9-1-7-3)10-2-8-4/h1-2H,(H3,6,7,8,9,10)
InchiKey:	GFFGJBXGBJISGV-UHFFFAOYSA-N
Formula:	C5H5N5
SMILES:	Nc1ncnc2[nH]cnc12
Mol. weight [g/mol]:	135.13
CAS:	73-24-5

Physical Properties

Property code	Value	Unit	Source
affp	942.80	kJ/mol	NIST Webbook
basg	912.50	kJ/mol	NIST Webbook
chs	-2778.10 ± 0.88	kJ/mol	NIST Webbook
chs	-2779.00 ± 1.30	kJ/mol	NIST Webbook
ea	0.01 ± 0.01	eV	NIST Webbook
hfs	96.02 ± 0.92	kJ/mol	NIST Webbook

hfs	96.90 ± 1.30	kJ/mol	NIST Webbook
hsub	110.00	kJ/mol	NIST Webbook
ie	8.90 ± 0.10	eV	NIST Webbook
ie	8.48	eV	NIST Webbook
ie	8.48	eV	NIST Webbook
ie	8.30 ± 0.10	eV	NIST Webbook
ie	8.44 ± 0.03	eV	NIST Webbook
log10ws	-2.12		Estimated Solubility Method
log10ws	-2.43		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-2.10		Aqueous Solubility Prediction Method
logp	-0.547		Crippen Method
mcvol	92.290	ml/mol	McGowan Method
rinpol	1836.00		NIST Webbook
ss	151.01	J/mol×K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	147.00	J/mol×K	298.00	NIST Webbook
cps	143.13	J/mol×K	298.10	NIST Webbook
hsubt	109.20	kJ/mol	460.50	NIST Webbook
hsubt	127.20 ± 1.90	kJ/mol	421.00	NIST Webbook
rhol	1088.40	kg/m3	313.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis
rhol	1094.50	kg/m3	303.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis

rhol	1091.40	kg/m3	308.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis
rhol	1097.60	kg/m3	298.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis
rhol	1085.30	kg/m3	318.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis
rhol	1082.30	kg/m3	323.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis
rhol	1079.30	kg/m3	328.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis
rhol	1076.20	kg/m3	333.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis
rhol	1073.30	kg/m3	338.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis

rhol	1070.30	kg/m3	343.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis

Sources

Solubility modelling and preferential solvation of adenine in solvent mixtures of (N,N-dimethylformamide, N-methyl pyrrolidone, propylene glycol and dimethyl sulfoxide) plus water:	https://www.doi.org/10.1016/j.jct.2018.05.030
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C73245&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis:	https://www.doi.org/10.1016/j.jct.2012.07.022

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
ea:	Electron affinity
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ss:	Solid phase molar entropy at standard conditions