9H-PURIN-6-YLAMINE

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 adenine
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

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	8.44 ± 0.03	eV	NIST Webbook
ie	8.48	eV	NIST Webbook
ie	8.48	eV	NIST Webbook
ie	8.90 ± 0.10	eV	NIST Webbook
ie	8.30 ± 0.10	eV	NIST Webbook
log10ws	-2.10		Aqueous Solubility Prediction Method
log10ws	-2.43		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-2.12		Estimated Solubility 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
tf	572.17	K	Cheméo Relay (1.0)

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	127.20 ± 1.90	kJ/mol	421.00	NIST Webbook
hsubt	109.20	kJ/mol	460.50	NIST Webbook
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	1082.30	kg/m3	323.15	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	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
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	1088.40	kg/m3	313.15	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	1094.50	kg/m3	303.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis

Sources

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
Thermodynamics of aqueous adenine: Standard partial molar volumes and heat capacities of adenine, adeninium chloride, and sodium adeninate from T = 283.15 K to 363.15 K:	https://www.doi.org/10.1016/j.jct.2017.04.005
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
Cheméo Relay (1.0, beta):	
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C73245&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0):	

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

tf: Normal melting (fusion) point