3-Aminopyridine

Other names:	.beta.-aminopyridine
	3-pyridinamine
	3-pyridylamine
	Amino-3 pyridine
	UN 2671
	m-Aminopyridine
	pyridine, 3-amino-
	«beta»-Aminopyridine
Inchi:	InChI=1S/C5H6N2/c6-5-2-1-3-7-4-5/h1-4H,6H2
InchiKey:	CUYKNJBYIJFRCU-UHFFFAOYSA-N
Formula:	C5H6N2
SMILES:	Nc1cccnc1
Mol. weight [g/mol]:	94.11
CAS:	462-08-8

Physical Properties

Property code	Value	Unit	Source
affp	954.40	kJ/mol	NIST Webbook
basg	922.60	kJ/mol	NIST Webbook
chs	-2885.20 ± 0.50	kJ/mol	NIST Webbook
hf	144.20 ± 1.60	kJ/mol	NIST Webbook
hfs	60.20 ± 0.80	kJ/mol	NIST Webbook
hsub	84.00 ± 1.40	kJ/mol	NIST Webbook
hsub	84.00	kJ/mol	NIST Webbook
hsub	80.70 ± 0.30	kJ/mol	NIST Webbook
hsub	84.00 ± 1.40	kJ/mol	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	8.70 ± 0.10	eV	NIST Webbook
ie	9.03 ± 0.05	eV	NIST Webbook
ie	8.44	eV	NIST Webbook
log10ws	-0.87		Crippen Method
logp	0.664		Crippen Method
mcvol	77.510	ml/mol	McGowan Method
rinpol	1105.00		NIST Webbook
rinpol	1105.00		NIST Webbook
ripol	2125.00		NIST Webbook
ripol	2111.00		NIST Webbook

ripol	2156.00		NIST Webbook
ripol	2143.00		NIST Webbook
ripol	2142.00		NIST Webbook
ripol	2122.00		NIST Webbook
tb	520.00 ± 1.00	K	NIST Webbook
tb	525.20	K	NIST Webbook
tb	524.00 ± 1.00	K	NIST Webbook
tb	521.20	K	NIST Webbook
tf	337.65 ± 0.20	K	NIST Webbook
tf	337.15 ± 1.50	K	NIST Webbook
tf	337.00	K	NIST Webbook
tf	337.65	K	Effect of temperature on the solubility of 3-aminopyridine in binary ethanol + toluene solvent mixtures
tf	337.65	K	Solubility of 3-Aminopyridine in Acetone + n-Butyl Acetate from (288.15 to 323.15) K

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	14.40	kJ/mol	335.50	NIST Webbook

Sources

Solubility of 3-Aminopyridine in Acetone + n-Butyl Acetate from (288.15 to 323.15) K:	https://www.doi.org/10.1021/je800945e
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C462088&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Effect of temperature on the solubility of 3-aminopyridine in binary ethanol + toluene solvent mixtures:	https://www.doi.org/10.1016/j.fluid.2011.11.023

Legend

affp: Proton affinity

basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point