

4-Aminopyridine

Other names:	Fampridine 4-Pyridinamine Pyridine, 4-amino- «gamma»-Aminopyridine p-Aminopyridine Phillips 1861 VMI 10-3 4-Pyridylamine Amino-4 pyridine Avitrol Avitrol 200 Compound 1861 Pimadin (free base) Prc 1237 4-AP Rcra waste number P008 NSC 15041 Frampridine
Inchi:	InChI=1S/C5H6N2/c6-5-1-3-7-4-2-5/h1-4H,(H2,6,7)
InchiKey:	NUKYPUAOHBNCYPY-UHFFFAOYSA-N
Formula:	C5H6N2
SMILES:	<chem>Nc1ccncc1</chem>
Mol. weight [g/mol]:	94.11
CAS:	504-24-5

Physical Properties

Property code	Value	Unit	Source
affp	979.70	kJ/mol	NIST Webbook
basg	947.80	kJ/mol	NIST Webbook
chs	-2866.80 ± 0.50	kJ/mol	NIST Webbook
hf	129.90 ± 1.40	kJ/mol	NIST Webbook
hfs	41.80 ± 0.80	kJ/mol	NIST Webbook
hsub	88.10 ± 1.10	kJ/mol	NIST Webbook
hsub	87.10 ± 0.40	kJ/mol	NIST Webbook
hsub	88.10	kJ/mol	NIST Webbook
hsub	88.10 ± 1.10	kJ/mol	NIST Webbook
ie	8.97 ± 0.05	eV	NIST Webbook

ie	8.76	eV	NIST Webbook
ie	8.77	eV	NIST Webbook
ie	8.80 ± 0.10	eV	NIST Webbook
ie	9.27 ± 0.05	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
log10ws	-0.87		Crippen Method
logp	0.664		Crippen Method
mcvol	77.510	ml/mol	McGowan Method
ripol	1158.00		NIST Webbook
ripol	1158.00		NIST Webbook
ripol	1170.00		NIST Webbook
ripol	1158.00		NIST Webbook
ripol	2287.00		NIST Webbook
ripol	2278.00		NIST Webbook
ripol	2325.00		NIST Webbook
ripol	2324.00		NIST Webbook
ripol	2298.00		NIST Webbook
ripol	2287.00		NIST Webbook
ripol	2300.00		NIST Webbook
ripol	2278.00		NIST Webbook
tb	546.20	K	NIST Webbook
tf	432.65 ± 1.00	K	NIST Webbook
tf	432.15 ± 0.50	K	NIST Webbook
tf	431.00	K	NIST Webbook
tf	431.98 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	20.07	kJ/mol	429.90	NIST Webbook
hfust	20.07	kJ/mol	429.90	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	453.00	K	1.60	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C504245&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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