

Pyridine, 4-(methylthio)-

Other names:	4-(Methylthio)pyridine
Inchi:	InChI=1S/C6H7NS/c1-8-6-2-4-7-5-3-6/h2-5H,1H3
InchiKey:	XCHSSZMKKXPBAI-UHFFFAOYSA-N
Formula:	C6H7NS
SMILES:	CSc1ccncc1
Mol. weight [g/mol]:	125.19
CAS:	22581-72-2

Physical Properties

Property code	Value	Unit	Source
affp	955.20	kJ/mol	NIST Webbook
basg	923.30	kJ/mol	NIST Webbook
ie	9.00 ± 0.02	eV	NIST Webbook
ie	8.73 ± 0.03	eV	NIST Webbook
log10ws	-1.98		Crippen Method
logp	1.804		Crippen Method
mcvol	97.970	ml/mol	McGowan Method
ripol	1796.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	75.30 ± 3.80	kJ/mol	365.00	NIST Webbook
hvapt	55.80	kJ/mol	364.50	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22581722&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
hsubt:	Enthalpy of sublimation at a given temperature
hvapt:	Enthalpy of vaporization 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
ripol:	Polar retention indices

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