Pyridine, 3-(methylthio)-

Other names: 3-(Methylthio)pyridine
Inchi: InChI=1S/C6H7NS/c1-8-6-3-2-4-7-5-6/h2-5H,1H3
InchiKey: AULOGPOZBOCNSX-UHFFFAOYSA-N
Formula: C6H7NS
SMILES: CSc1cccnc1
Mol. weight [g/mol]: 125.19
CAS: 18794-33-7

Physical Properties

Property code	Value	Unit	Source
affp	936.50	kJ/mol	NIST Webbook
basg	904.70	kJ/mol	NIST Webbook
ie	8.93 ± 0.02	eV	NIST Webbook
ie	8.41 ± 0.03	eV	NIST Webbook
log10ws	-1.98		Crippen Method
logp	1.804		Crippen Method
mcvol	97.970	ml/mol	McGowan Method
rinpol	1152.00		NIST Webbook
rinpol	1152.00		NIST Webbook
ripol	1791.00		NIST Webbook
ripol	1791.00		NIST Webbook
ripol	1803.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18794337&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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