4(1H)-Pyridinethione,1-methyl-

Inchi: InChI=1S/C6H7NS/c1-7-4-2-6(8)3-5-7/h2-5H,1H3
InchiKey: AXSKLZVLVONUIC-UHFFFAOYSA-N
Formula: C6H7NS
SMILES: Cn1ccc(=S)cc1
Mol. weight [g/mol]: 125.19
CAS: 6887-59-8

Physical Properties

Property code	Value	Unit	Source
hvap	172.00 ± 8.40	kJ/mol	NIST Webbook
ie	7.54 ± 0.02	eV	NIST Webbook
ie	7.60 ± 0.03	eV	NIST Webbook
log10ws	-3.61		Crippen Method
logp	1.755		Crippen Method
mcvol	97.970	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	188.30 ± 9.20	kJ/mol	452.50	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6887598&Units=SI

Legend

hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume