3-Pyridinol, 2-(methylthio)-

Inchi: InChI=1S/C6H7NOS/c1-9-6-5(8)3-2-4-7-6/h2-4,8H,1H3
InchiKey: LZMQEAWZBGDJCE-UHFFFAOYSA-N
Formula: C6H7NOS
SMILES: CSc1ncccc1O
Mol. weight [g/mol]: 141.19
CAS: 32637-37-9

Physical Properties

Property code	Value	Unit	Source
ie	8.53 ± 0.05	eV	NIST Webbook
log10ws	-1.53		Crippen Method
logp	1.509		Crippen Method
mcvol	103.840	ml/mol	McGowan Method
ripol	1805.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C32637379&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

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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