2-(Methylthio)methylpyridine

Inchi: InChI=1S/C7H9NS/c1-9-6-7-4-2-3-5-8-7/h2-5H,6H2,1H3
InchiKey: KWXDPVBKJYKQIM-UHFFFAOYSA-N
Formula: C7H9NS
SMILES: CSCc1ccccn1
Mol. weight [g/mol]: 139.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.42		Crippen Method
logp	1.945		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
ripol	1990.00		NIST Webbook
ripol	1990.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R319716&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

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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