

3-[(methylthio)methyl]pyridine

Inchi:	InChI=1S/C7H9NS/c1-9-6-7-3-2-4-8-5-7/h2-5H,6H2,1H3
InchiKey:	DMBKVOYJOGETRJ-UHFFFAOYSA-N
Formula:	C7H9NS
SMILES:	CSCc1cccnc1
Mol. weight [g/mol]:	139.22
CAS:	69966-44-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.42		Crippen Method
logp	1.945		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
rinpol	1243.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69966445&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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