3-(Methylaminomethyl)pyridine

Inchi: InChI=1S/C7H10N2/c1-8-5-7-3-2-4-9-6-7/h2-4,6,8H,5H2,1H3
InchiKey: MCSAQVGDZLPTBS-UHFFFAOYSA-N
Formula: C7H10N2
SMILES: CNCc1cccnc1
Mol. weight [g/mol]: 122.17
CAS: 20173-04-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.72		Crippen Method
logp	0.801		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
rinpol	1111.40		NIST Webbook

Sources

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=C20173040&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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