6-(2-Methoxyethyl)-2-picoline

Inchi: InChI=1S/C9H13NO/c1-8-4-3-5-9(10-8)6-7-11-2/h3-5H,6-7H2,1-2H3
InchiKey: ZKQBRFRQZNYNQI-UHFFFAOYSA-N
Formula: C9H13NO
SMILES: COCCc1cccc(C)n1
Mol. weight [g/mol]: 151.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.02		Crippen Method
logp	1.579		Crippen Method
mcvol	129.760	ml/mol	McGowan Method
rinpol	1144.20		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R264829&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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