1-(2-Methoxyethyl)pyridinium

Inchi: InChI=1S/C8H12NO/c1-10-8-7-9-5-3-2-4-6-9/h2-6H,7-8H2,1H3/q+1
InchiKey: LOPCHXHUZUVFEV-UHFFFAOYSA-N
Formula: C8H12NO
SMILES: COCC[n+]1ccccc1
Mol. weight [g/mol]: 138.19
CAS: 125713-87-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Crippen Method
logp	0.621		Crippen Method
mcvol	117.820	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C125713873&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

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