2-(2-resp-3-methyl-1-pyrrolyl)ethan-l-ol

Inchi: InChI=1S/C7H11NO/c1-7-3-2-4-8(7)5-6-9/h2-4,9H,5-6H2,1H3
InchiKey: FBKRNPLLIWQEPY-UHFFFAOYSA-N
Formula: C7H11NO
SMILES: Cc1cccn1CCO
Mol. weight [g/mol]: 125.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.47		Crippen Method
logp	0.789		Crippen Method
mcvol	105.880	ml/mol	McGowan Method
ripol	1991.00		NIST Webbook
ripol	1991.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R296712&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
ripol: Polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.