3-(3-resp-2-methyl-1-pyrrolyl)propanol

Inchi: InChI=1S/C8H13NO/c1-8-4-2-5-9(8)6-3-7-10/h2,4-5,10H,3,6-7H2,1H3
InchiKey: MJLJQQATDBLMEE-UHFFFAOYSA-N
Formula: C8H13NO
SMILES: Cc1cccn1CCCO
Mol. weight [g/mol]: 139.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.89		Crippen Method
logp	1.179		Crippen Method
mcvol	119.970	ml/mol	McGowan Method
ripol	1917.00		NIST Webbook
ripol	1917.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R296876&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
ripol: Polar retention indices

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