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

Inchi: InChI=1S/C8H13NO/c1-8-3-5-9(7-8)4-2-6-10/h3,5,7,10H,2,4,6H2,1H3
InchiKey: JWFUEAIBMBPCBK-UHFFFAOYSA-N
Formula: C8H13NO
SMILES: Cc1ccn(CCCO)c1
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	1883.00		NIST Webbook
ripol	1883.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R296861&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

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