2-(1-pyrrolyl)-1-ethanol

Other names: 2-(1-pyrrolyl)ethan-1-ol
Inchi: InChI=1S/C6H9NO/c8-6-5-7-3-1-2-4-7/h1-4,8H,5-6H2
InchiKey: ZIOLCZCJJJNOEJ-UHFFFAOYSA-N
Formula: C6H9NO
SMILES: OCCn1cccc1
Mol. weight [g/mol]: 111.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.00		Crippen Method
logp	0.480		Crippen Method
mcvol	91.790	ml/mol	McGowan Method
ripol	1935.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R296698&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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