

1-(1-pyrrolyl)propan-2-ol

Inchi: InChI=1S/C7H11NO/c1-7(9)6-8-4-2-3-5-8/h2-5,7,9H,6H2,1H3
InchiKey: UJMFUOHZAQFYCK-UHFFFAOYSA-N
Formula: C7H11NO
SMILES: CC(O)Cn1cccc1
Mol. weight [g/mol]: 125.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.53		Crippen Method
logp	0.869		Crippen Method
mcvol	105.880	ml/mol	McGowan Method
ripol	1828.00		NIST Webbook
ripol	1828.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R296856&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

Latest version available from:

<https://www.chemeo.com/cid/92-719-2/1-1-pyrrolyl-propan-2-ol.pdf>

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