2-(1-pyrrolidinyl)-3-pentanone

Inchi: InChI=1S/C9H17NO/c1-3-9(11)8(2)10-6-4-5-7-10/h8H,3-7H2,1-2H3
InchiKey: URXJQXJRZXGXTQ-UHFFFAOYSA-N
Formula: C9H17NO
SMILES: CCC(=O)C(C)N1CCCC1
Mol. weight [g/mol]: 155.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.45		Crippen Method
logp	1.450		Crippen Method
mcvol	138.360	ml/mol	McGowan Method
ripol	1490.00		NIST Webbook
ripol	1490.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R312166&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

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