3-(1'-pyrrolidinyl)-2-butanone

Other names: 3-(1-pyrrolidinyl)-2-butanone
Inchi: InChI=1S/C8H15NO/c1-7(8(2)10)9-5-3-4-6-9/h7H,3-6H2,1-2H3
InchiKey: IXYTUYCLJBLYKD-UHFFFAOYSA-N
Formula: C8H15NO
SMILES: CC(=O)C(C)N1CCCC1
Mol. weight [g/mol]: 141.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.03		Crippen Method
logp	1.060		Crippen Method
mcvol	124.270	ml/mol	McGowan Method
ripol	1420.00		NIST Webbook
ripol	1420.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U366037&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices