2-Hydroxy-1-(1'-pyrrolidinyl)-1-buten-3-one

Other names: 2-Hydroxy-1-(1-pyrrolidinyl)-1-buten-3-one
Inchi: InChI=1S/C8H13NO2/c1-7(10)8(11)6-9-4-2-3-5-9/h6,11H,2-5H2,1H3/b8-6-
InchiKey: BVQIJAGLTDWTAU-VURMDHGXSA-N
Formula: C8H13NO2
SMILES: CC(=O)C(O)=CN1CCCC1
Mol. weight [g/mol]: 155.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.08		Crippen Method
logp	1.071		Crippen Method
mcvol	125.840	ml/mol	McGowan Method
ripol	2459.00		NIST Webbook
ripol	2459.00		NIST Webbook

Sources

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=R77507&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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