2-acetyl-1-ethylpyrrole

Inchi: InChI=1S/C8H11NO/c1-3-9-6-4-5-8(9)7(2)10/h4-6H,3H2,1-2H3
InchiKey: HQADRFRTIALOCB-UHFFFAOYSA-N
Formula: C8H11NO
SMILES: CCn1cccc1C(C)=O
Mol. weight [g/mol]: 137.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	1.711		Crippen Method
mcvol	115.670	ml/mol	McGowan Method
ripol	1635.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R321576&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