2-acetyl-N-isobutenyl-pyrrole

Inchi: InChI=1S/C10H13NO/c1-8(2)7-11-6-4-5-10(11)9(3)12/h4-7H,1-3H3
InchiKey: INPDUHMRCHDTIC-UHFFFAOYSA-N
Formula: C10H13NO
SMILES: CC(=O)c1cccn1C=C(C)C
Mol. weight [g/mol]: 163.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.25		Crippen Method
logp	2.571		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
ripol	1874.00		NIST Webbook
ripol	1874.00		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=R314731&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.