

2-acetyl-N-isobutylpyrrole

Inchi: InChI=1S/C10H15NO/c1-8(2)7-11-6-4-5-10(11)9(3)12/h4-6,8H,7H2,1-3H3
InchiKey: MADPUDKSZYVYKP-UHFFFAOYSA-N
Formula: C10H15NO
SMILES: CC(=O)c1cccn1CC(C)C
Mol. weight [g/mol]: 165.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.99		Crippen Method
logp	2.347		Crippen Method
mcvol	143.850	ml/mol	McGowan Method
ripol	1700.00		NIST Webbook
ripol	1700.00		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=R314746&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

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<https://www.chemeo.com/cid/85-700-0/2-acetyl-N-isobutylpyrrole.pdf>

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