Pyridine, 2-acetyl-4-(1-methylethyl)

Inchi: InChI=1S/C10H13NO/c1-7(2)9-4-5-11-10(6-9)8(3)12/h4-7H,1-3H3
InchiKey: BWJDKYNJXZATRV-UHFFFAOYSA-N
Formula: C10H13NO
SMILES: CC(=O)c1cc(C(C)C)ccn1
Mol. weight [g/mol]: 163.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Crippen Method
logp	2.408		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
rinpol	1260.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1260.00		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=R68633&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices