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

Inchi: InChI=1S/C10H11NO/c1-7(2)9-4-5-11-10(6-9)8(3)12/h4-6H,1H2,2-3H3
InchiKey: QGALSOGFUDWZMF-UHFFFAOYSA-N
Formula: C10H11NO
SMILES: C=C(C)c1ccnc(C(C)=O)c1
Mol. weight [g/mol]: 161.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.14		Crippen Method
logp	2.317		Crippen Method
mcvol	135.250	ml/mol	McGowan Method
rinpol	1323.00		NIST Webbook
rinpol	1323.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R68629&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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