

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

Inchi: InChI=1S/C10H11NO/c1-7(2)10-6-9(8(3)12)4-5-11-10/h4-6H,1H2,2-3H3
InchiKey: RYNRLVOZUDLPQK-UHFFFAOYSA-N
Formula: C10H11NO
SMILES: C=C(C)c1cc(C(C)=O)ccn1
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	1331.00		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1331.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R68722&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

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<https://www.chemeo.com/cid/38-332-1/Pyridine-4-acetyl-2-1-methylethenyl.pdf>

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