2-acetyl-4(3)-methylpyrrole

Inchi: InChI=1S/C7H9NO/c1-5-3-7(6(2)9)8-4-5/h3-4,8H,1-2H3
InchiKey: FTZSIAYCTJFZPV-UHFFFAOYSA-N
Formula: C7H9NO
SMILES: CC(=O)c1cc(C)c[nH]1
Mol. weight [g/mol]: 123.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.83		Crippen Method
logp	1.044		Crippen Method
mcvol	101.580	ml/mol	McGowan Method
ripol	2036.00		NIST Webbook
ripol	2036.00		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=R296787&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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