2-Methoxy-1,6-dimethyl-4-pyridone

Inchi: InChI=1S/C8H11NO2/c1-6-4-7(10)5-8(11-3)9(6)2/h4-5H,1-3H3
InchiKey: PJKZMGMLGHZFJO-UHFFFAOYSA-N
Formula: C8H11NO2
SMILES: COc1cc(=O)cc(C)n1C
Mol. weight [g/mol]: 153.18
CAS: 40334-98-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.78		Crippen Method
logp	0.702		Crippen Method
mcvol	121.540	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40334983&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume