2,4-Dimethyl-1H-pyrrole-5-carboxylic acid methyl ester

Inchi: InChI=1S/C8H11NO2/c1-5-4-6(2)9-7(5)8(10)11-3/h4,9H,1-3H3
InchiKey: NNDPBEVKFHCFGQ-UHFFFAOYSA-N
Formula: C8H11NO2
SMILES: COC(=O)c1[nH]c(C)cc1C
Mol. weight [g/mol]: 153.18
CAS: 74999-36-3

Physical Properties

Property code	Value	Unit	Source
chs	-4307.00	kJ/mol	NIST Webbook
log10ws	-1.88		Crippen Method
logp	0.936		Crippen Method
mcvol	121.540	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C74999363&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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