1H-Pyrrole-2-carboxylic acid, 4,5-dimethyl-, ethyl ester

Other names: 4,5-Dimethyl-1H-pyrrole-2-carboxylic acid ethyl ester
Inchi: InChI=1S/C9H13NO2/c1-4-12-9(11)8-5-6(2)7(3)10-8/h5,10H,4H2,1-3H3
InchiKey: NJUXFNQDUIJYPO-UHFFFAOYSA-N
Formula: C9H13NO2
SMILES: CCOC(=O)c1cc(C)c(C)[nH]1
Mol. weight [g/mol]: 167.21
CAS: 2199-45-3

Physical Properties

Property code	Value	Unit	Source
chs	-4950.10 ± 5.00	kJ/mol	NIST Webbook
hfs	-449.40 ± 5.00	kJ/mol	NIST Webbook
log10ws	-2.30		Crippen Method
logp	1.326		Crippen Method
mcvol	135.630	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=C2199453&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
hfs: Solid phase enthalpy of formation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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