1H-Pyrrole-2-carboxylic acid, 3,5-dimethyl-, ethyl ester

Other names: 3,5-Dimethyl-1H-pyrrole-2-carboxylic acid ethyl ester
Ethyl 3,5-dimethyl-2-pyrrolecarboxylate
Pyrrole-2-carboxylic acid, 3,5-dimethyl-, ethyl ester
ethyl 3,5-dimethyl-1H-pyrrole-2-carboxylate

Inchi: InChI=1S/C9H13NO2/c1-4-12-9(11)8-6(2)5-7(3)10-8/h5,10H,4H2,1-3H3

InchiKey: IZSBSZYFPYIJDI-UHFFFAOYSA-N

Formula: C9H13NO2

SMILES: CCOC(=O)c1[nH]c(C)cc1C

Mol. weight [g/mol]: 167.21

CAS: 2199-44-2

Physical Properties

Property code	Value	Unit	Source
chs	-4925.00 ± 5.00	kJ/mol	NIST Webbook
hfs	-474.50 ± 5.00	kJ/mol	NIST Webbook
ie	7.91	eV	NIST Webbook
log10ws	-2.62		Aqueous Solubility Prediction Method
logp	1.326		Crippen Method
mcvol	135.630	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.70	K	1.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2199442&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure