

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

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=C2199453&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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