

# 2,4,5-Trimethyl-1H-pyrrole-3-carboxylic acid ethyl ester

**Other names:** Pyrrole-3-carboxylic acid, 2,4,5-trimethyl-, ethyl ester  
**Inchi:** InChI=1S/C10H15NO2/c1-5-13-10(12)9-6(2)7(3)11-8(9)4/h11H,5H2,1-4H3  
**InchiKey:** WAPMICOPEJJCJAD-UHFFFAOYSA-N  
**Formula:** C10H15NO2  
**SMILES:** CCOC(=O)c1c(C)[nH]c(C)c1C  
**Mol. weight [g/mol]:** 181.23  
**CAS:** 2199-54-4

## Physical Properties

Property code	Value	Unit	Source
chs	-5589.00 ± 5.40	kJ/mol	NIST Webbook
log10ws	-2.78		Crippen Method
logp	1.635		Crippen Method
mcvol	149.720	ml/mol	McGowan Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2199544&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## 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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