

# 1H-Pyrrole-2,4-dicarboxylic acid, 3,5-dimethyl-, diethyl ester

Other names:

Pyrrole-2,4-dicarboxylic acid, 3,5-dimethyl-, diethyl ester

Diethyl 3,5-dimethylpyrrole-2,4-dicarboxylate

Knorr's pyrrole

2,4-Dimethyl-3,5-dicarbethoxypyrrole

3,5-Dimethyl-1H-pyrrole-2,4-dicarboxylic acid diethyl ester

2,4-Dimethyl-3,5-diethoxycarbonyl-pyrrole

Diethyl 2,4-dimethylpyrrole-3,5-dicarboxylate

Pyrrole-3,5-bis(carboxylic acid), 2,4-dimethyl-, diethyl ester

**Inchi:** InChI=1S/C12H17NO4/c1-5-16-11(14)9-7(3)10(13-8(9)4)12(15)17-6-2/h13H,5-6H2,1-4H

**InchiKey:** XSBSXJAYEPDGSF-UHFFFAOYSA-N

**Formula:** C12H17NO4

**SMILES:** CCOC(=O)c1[nH]c(C)c(C(=O)OCC)c1C

**Mol. weight [g/mol]:** 239.27

**CAS:** 2436-79-5

## Physical Properties

Property code	Value	Unit	Source
chs	-6235.00 ± 6.30	kJ/mol	NIST Webbook
hfs	-916.70 ± 6.30	kJ/mol	NIST Webbook
ie	8.15	eV	NIST Webbook
log10ws	-2.96		Crippen Method
logp	1.503		Crippen Method
mcvol	185.340	ml/mol	McGowan Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2436795&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

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

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