

1H-Pyrrole-2-carboxylic acid, 3,4,5-trimethyl, ethyl ester

Other names:	Ethyl 3,4,5-trimethylpyrrole-2-carboxylate Pyrrole-2-carboxylic acid, 3,4,5-trimethyl-, ethyl ester Ethyl 3,4,5-trimethyl-1H-pyrrole-2-carboxylate
Inchi:	InChI=1S/C10H15NO2/c1-5-13-10(12)9-7(3)6(2)8(4)11-9/h11H,5H2,1-4H3
InchiKey:	WBOGFZDTCIQHSX-UHFFFAOYSA-N
Formula:	C10H15NO2
SMILES:	CCOC(=O)c1[nH]c(C)c(C)c1C
Mol. weight [g/mol]:	181.23
CAS:	2199-46-4

Physical Properties

Property code	Value	Unit	Source
ie	7.71	eV	NIST Webbook
log10ws	-2.78		Crippen Method
logp	1.635		Crippen Method
mcvol	149.720	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2199464&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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