Ethyl 3,4,5-trimethylpyrrole-2-carboxylate

Other names:	Ethyl 3,4,5-trimethyl-1H-pyrrole-2-carboxylate
	Ethyl 3,4,5-trimethylpyrrole-2-carboxylate
	Pyrrole-2-carboxylic acid, 3,4,5-trimethyl-, ethyl ester
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]:	181.24

Physical Properties

Property code	Value	Unit	Source
hf	-408.60	kJ/mol	Cheméo Relay (1.0)
hvap	74.26	kJ/mol	Cheméo Relay (1.0)
ie	7.71	eV	NIST Webbook
log10ws	-2.86		Cheméo Relay (1.0)
logp	1.635		Crippen Method
mcvol	149.720	ml/mol	McGowan Method
pc	2483.51	kPa	Cheméo Relay (1.0, beta)
tb	541.64	K	Cheméo Relay (1.0)
tf	377.38	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2199464&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point