3,5-dimethyl-4-propyl-1H-pyrrole-2-carboxylic acid ethyl ester

Inchi: InChI=1S/C12H19NO2/c1-5-7-10-8(3)11(13-9(10)4)12(14)15-6-2/h13H,5-7H2,1-4H3
InchiKey: FURNFZQCOQEXNH-UHFFFAOYSA-N
Formula: C12H19NO2
SMILES: CCCc1c(C)[nH]c(C(=O)OCC)c1C
Mol. weight [g/mol]: 209.29

Physical Properties

Property code	Value	Unit	Source
chs	-6868.50 ± 2.10	kJ/mol	NIST Webbook
ie	7.87	eV	Cheméo Relay (1.0)
log10ws	-3.65		Cheméo Relay (1.0)
logp	2.279		Crippen Method
mcvol	177.900	ml/mol	McGowan Method

Sources

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4758649&Units=SI

Legend

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