

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]:	209.28
CAS:	4758-64-9

Physical Properties

Property code	Value	Unit	Source
chs	-6868.50 ± 2.10	kJ/mol	NIST Webbook
log10ws	-3.52		Crippen Method
logp	2.279		Crippen Method
mcvol	177.900	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=C4758649&Units=SI

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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