2,4-Dimethyl-5-hydroxy-1H-pyrrol-3-carboxylic acid ethyl ester

Inchi: InChI=1S/C9H13NO3/c1-4-13-9(12)7-5(2)8(11)10-6(7)3/h10-11H,4H2,1-3H3
InchiKey: JNQZBAQUMFAVOI-UHFFFAOYSA-N
Formula: C9H13NO3
SMILES: CCOC(=O)c1c(C)[nH]c(O)c1C
Mol. weight [g/mol]: 183.20
CAS: 4030-28-8

Physical Properties

Property code	Value	Unit	Source
chs	-4714.90 ± 4.60	kJ/mol	NIST Webbook
log10ws	-1.85		Crippen Method
logp	1.032		Crippen Method
mcvol	141.500	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4030288&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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