4-Ethyl-3,5-dimethyl-1H-pyrrole-2-carboxaldehyde

Other names: 1H-Pyrrole-2-carboxaldehyde, 4-ethyl-3,5-dimethyl-
1H-Pyrrole-2-carbaldehyde, 4-ethyl-3,5-dimethyl-
Inchi: InChI=1S/C9H13NO/c1-4-8-6(2)9(5-11)10-7(8)3/h5,10H,4H2,1-3H3
InchiKey: VHIKIUXLJPZNCA-UHFFFAOYSA-N
Formula: C9H13NO
SMILES: CCc1c(C)[nH]c(C=O)c1C
Mol. weight [g/mol]: 151.21
CAS: 6250-80-2

Physical Properties

Property code	Value	Unit	Source
chs	-5144.60 ± 5.00	kJ/mol	NIST Webbook
hfs	-254.80 ± 5.00	kJ/mol	NIST Webbook
log10ws	-2.69		Crippen Method
logp	1.525		Crippen Method
mcvol	129.760	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6250802&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
hfs: Solid phase enthalpy of formation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume