Pyrrole-3-carboxylic acid, 2,4,5-trimethyl-, ethyl ester

Other names: Pyrrole-3-carboxylic acid, 2,4,5-trimethyl-, ethyl ester
Inchi: InChI=1S/C10H15NO2/c1-5-13-10(12)9-6(2)7(3)11-8(9)4/h11H,5H2,1-4H3
InchiKey: WAPMICOPEJCJAD-UHFFFAOYSA-N
Formula: C10H15NO2
SMILES: CCOC(=O)c1c(C)[nH]c(C)c1C
Mol. weight [g/mol]: 181.24

Physical Properties

Property code	Value	Unit	Source
chs	-5589.00 ± 5.40	kJ/mol	NIST Webbook
hf	-404.53	kJ/mol	Cheméo Relay (1.0)
hvap	73.73	kJ/mol	Cheméo Relay (1.0)
ie	7.70	eV	Cheméo Relay (1.0)
log10ws	-2.58		Cheméo Relay (1.0)
logp	1.635		Crippen Method
mcvol	149.720	ml/mol	McGowan Method
pc	2471.71	kPa	Cheméo Relay (1.0, beta)
tb	535.23	K	Cheméo Relay (1.0)
tf	379.66	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2199544&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

chs:	Standard solid enthalpy of combustion
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