

1H-Pyrrole-2-carboxylic acid, 3,5-dimethyl-4-nitro-, ethyl ester

Other names:	Pyrrole-2-carboxylic acid, 3,5-dimethyl-4-nitro-, ethyl ester
Inchi:	InChI=1S/C9H12N2O4/c1-4-15-9(12)7-5(2)8(11(13)14)6(3)10-7/h10H,4H2,1-3H3
InchiKey:	AZGXAAUDJWAVHF-UHFFFAOYSA-N
Formula:	C9H12N2O4
SMILES:	CCOC(=O)c1[nH]c(C)c([N+](=O)[O-])c1C
Mol. weight [g/mol]:	212.20
CAS:	5463-44-5

Physical Properties

Property code	Value	Unit	Source
ie	8.76	eV	NIST Webbook
log10ws	-2.95		Crippen Method
logp	1.235		Crippen Method
mcvol	153.050	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=C5463445&Units=SI

Legend

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

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