

Nicotinic acid, 1,2-dihydro-4,6-dimethyl-5-nitro-2-oxo-, ethyl

Inchi:
ester

InChI=1S/C10H12N2O5/c1-4-17-10(14)7-5(2)8(12(15)16)6(3)11-9(7)13/h4H2,1-3H3,(H,1

InchiKey:

CSKMQCJKNCPERC-UHFFFAOYSA-N

Formula:

C10H12N2O5

SMILES:

CCOC(=O)c1c(C)c([N+](=O)[O-])c(C)[nH]c1=O

Mol. weight [g/mol]:

240.21

CAS:

6972-37-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.38		Crippen Method
logp	0.595		Crippen Method
mcvol	168.710	ml/mol	McGowan Method

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C6972378&Units=SI>

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>

Legend

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

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