

1H-Pyrazole-3-carboxylic acid, 4,5-dihydro-5-oxo-1-phenyl-, ethyl ester

Other names:

1-Phenyl-3-carbethoxypyrazolone
2-Pyrazoline-3-carboxylic acid, 5-oxo-1-phenyl-, ethyl ester
3-(Ethoxycarbonyl)-1-phenyl-5-pyrazolone
1-Phenyl-5-oxo-2-pyrazoline-3-carboxylic acid, ethyl ester
ethyl 5-oxo-1-phenyl-2-pyrazoline-3-carboxylate

Inchi:

InChI=1S/C12H12N2O3/c1-2-17-12(16)10-8-11(15)14(13-10)9-6-4-3-5-7-9/h3-7H,2,8H2,

InchiKey:

WBFXQKNQVZMOSQ-UHFFFAOYSA-N

Formula:

C12H12N2O3

SMILES:

CCOC(=O)C1=NN(c2ccccc2)C(=O)C1

Mol. weight [g/mol]:

232.24

CAS:

89-33-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.74		Crippen Method
logp	1.342		Crippen Method
mcvol	169.990	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=C89338&Units=SI>

Legend

log10ws:

Log10 of Water solubility in mol/l

logp:

Octanol/Water partition coefficient

mcvol:

McGowan's characteristic volume

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