

# Ethyl 3-amino-2-phenylpyrazole-4-carboxylate

**Other names:**

3-Amino-4-carbethoxy-2-phenylpyrazole  
5-Amino-4-carboethoxy-1-phenylpyrazole  
1H-Pyrazole-4-carboxylic acid, 5-amino-1-phenyl-, ethyl ester  
5-Amino-4-ethoxycarbonyl-1-phenylpyrazole  
ethyl 5-amino-1-phenyl-1H-pyrazole-4-carboxylate

**Inchi:**

InChI=1S/C12H13N3O2/c1-2-17-12(16)10-8-14-15(11(10)13)9-6-4-3-5-7-9/h3-8H,2,13H2

**InchiKey:**

AYJIUOZKKTUKKD-UHFFFAOYSA-N

**Formula:**

C12H13N3O2

**SMILES:**

CCOC(=O)c1cnn(-c2ccccc2)c1N

**Mol. weight [g/mol]:**

231.25

**CAS:**

16078-71-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.18		Crippen Method
logp	1.631		Crippen Method
mcvol	174.100	ml/mol	McGowan Method

## Sources

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C16078710&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](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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