

# 1H-Pyrazole-3-carboxylic acid, 5-methyl-, ethyl ester

<b>Other names:</b>	3(5)-Methyl-5(3)-ethoxycarbonylpyrazole 3-Ethoxycarbonyl-5-methylpyrazole ethyl 5-methyl-1H-pyrazole-3-carboxylate
<b>Inchi:</b>	InChI=1S/C7H10N2O2/c1-3-11-7(10)6-4-5(2)8-9-6/h4H,3H2,1-2H3,(H,8,9)
<b>InchiKey:</b>	BOTXQJAHRCGJEG-UHFFFAOYSA-N
<b>Formula:</b>	C7H10N2O2
<b>SMILES:</b>	CCOC(=O)c1cc(C)[nH]n1
<b>Mol. weight [g/mol]:</b>	154.17
<b>CAS:</b>	4027-57-0

## Physical Properties

Property code	Value	Unit	Source
affp	902.60	kJ/mol	NIST Webbook
basg	870.80	kJ/mol	NIST Webbook
log10ws	-1.59		Crippen Method
logp	0.413		Crippen Method
mcvol	117.430	ml/mol	McGowan Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4027570&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4027570&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

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