

# 3,5-diethoxycarbonylpyrazole

<b>Other names:</b>	1H-Pyrazole-3,5-dicarboxylic acid, 3,5-diethyl ester diethyl 3,5-pyrazoledicarboxylate
<b>Inchi:</b>	InChI=1S/C9H12N2O4/c1-3-14-8(12)6-5-7(11-10-6)9(13)15-4-2/h5H,3-4H2,1-2H3,(H,10,
<b>InchiKey:</b>	MBWXLICVQZUJOW-UHFFFAOYSA-N
<b>Formula:</b>	C9H12N2O4
<b>SMILES:</b>	CCOC(=O)c1cc(C(=O)OCC)[nH]n1
<b>Mol. weight [g/mol]:</b>	212.20
<b>CAS:</b>	37687-24-4

## Physical Properties

Property code	Value	Unit	Source
affp	881.60	kJ/mol	NIST Webbook
basg	849.70	kJ/mol	NIST Webbook
log10ws	-1.78		Crippen Method
logp	0.281		Crippen Method
mcvol	153.050	ml/mol	McGowan Method

## Sources

<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>
<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=C37687244&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C37687244&amp;Units=SI</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
<b>mcvol:</b>	McGowan's characteristic volume

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