

# Pyrazole-3,5-dicarboxylic acid, 1-methyl-, diethyl ester-

Other names:	1-Methyl-3,5-diethoxycarbonylpyrazole
Inchi:	InChI=1S/C10H14N2O4/c1-4-15-9(13)7-6-8(12(3)11-7)10(14)16-5-2/h6H,4-5H2,1-3H3
InchiKey:	WPKJUUKSWNCKPZ-UHFFFAOYSA-N
Formula:	C10H14N2O4
SMILES:	CCOC(=O)c1cc(C(=O)OCC)n(C)n1
Mol. weight [g/mol]:	226.23
CAS:	100852-80-0

## Physical Properties

Property code	Value	Unit	Source
affp	913.40	kJ/mol	NIST Webbook
basg	881.50	kJ/mol	NIST Webbook
log10ws	-3.85		Crippen Method
logp	0.773		Crippen Method
mcvol	167.140	ml/mol	McGowan Method

## Sources

NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C100852800&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C100852800&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

affp:	Proton affinity
basg:	Gas basicity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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