3,5-diethoxycarbonylpyrazole

Other names:	1H-Pyrazole-3,5-dicarboxylic acid, 3,5-diethyl ester
	diethyl 3,5-pyrazoledicarboxylate
Inchi:	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,
InchiKey:	MBWXLICVQZUJOW-UHFFFAOYSA-N
Formula:	C9H12N2O4
SMILES:	CCOC(=O)c1cc(C(=O)OCC)[nH]n1
Mol. weight [g/mol]:	212.20
CAS:	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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37687244&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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