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

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