1,3-dimethyl-5-ethoxycarbonylpyrazole

Inchi: InChI=1S/C8H12N2O2/c1-4-12-8(11)7-5-6(2)9-10(7)3/h5H,4H2,1-3H3
InchiKey: ZYSGPOXVDOROJU-UHFFFAOYSA-N
Formula: C8H12N2O2
SMILES: CCOC(=O)c1cc(C)nn1C
Mol. weight [g/mol]: 168.19
CAS: 5744-40-1

Physical Properties

Property code	Value	Unit	Source
affp	924.90	kJ/mol	NIST Webbook
basg	893.10	kJ/mol	NIST Webbook
log10ws	-3.66		Crippen Method
logp	0.905		Crippen Method
mcvol	131.520	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=C5744401&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