3(5)-phenyl-5(3)-ethoxycarbonylpyrazole

Inchi: InChI=1S/C12H12N2O2/c1-2-16-12(15)11-8-10(13-14-11)9-6-4-3-5-7-9/h3-8H,2H2,1H3,(
InchiKey: AZZHJDRWBMQEKD-UHFFFAOYSA-N
Formula: C12H12N2O2
SMILES: CCOC(=O)c1cc(-c2ccccc2)n[nH]1
Mol. weight [g/mol]: 216.24
CAS: 5932-30-9

Physical Properties

Property code	Value	Unit	Source
affp	899.70	kJ/mol	NIST Webbook
basg	867.80	kJ/mol	NIST Webbook
log10ws	-3.72		Crippen Method
logp	1.771		Crippen Method
mcvol	164.120	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5932309&Units=SI

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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