

1,5-dimethyl-3-ethoxycarbonylpyrazole

Inchi: InChI=1S/C8H12N2O2/c1-4-12-8(11)7-5-6(2)10(3)9-7/h5H,4H2,1-3H3
InchiKey: OJPXVXXMBWKEAT-UHFFFAOYSA-N
Formula: C8H12N2O2
SMILES: CCOC(=O)c1cc(C)n(C)n1
Mol. weight [g/mol]: 168.19
CAS: 5744-51-4

Physical Properties

Property code	Value	Unit	Source
affp	933.40	kJ/mol	NIST Webbook
basg	901.50	kJ/mol	NIST Webbook
log10ws	-3.66		Crippen Method
logp	0.905		Crippen Method
mcvol	131.520	ml/mol	McGowan Method

Sources

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=C5744514&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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