3H-Pyrazol-3-one, 2,4-dihydro-4,4,5-trimethyl-2-phenyl-

Other names: 2-Pyrazolin-5-one, 3,4,4-trimethyl-1-phenyl-
Inchi: InChI=1S/C12H14N2O/c1-9-12(2,3)11(15)14(13-9)10-7-5-4-6-8-10/h4-8H,1-3H3
InchiKey: MZYISAKYPPUWJG-UHFFFAOYSA-N
Formula: C12H14N2O
SMILES: CC1=NN(c2ccccc2)C(=O)C1(C)C
Mol. weight [g/mol]: 202.25
CAS: 947-82-0

Physical Properties

Property code	Value	Unit	Source
ie	7.50 ± 0.05	eV	NIST Webbook
ie	7.88 ± 0.05	eV	NIST Webbook
log10ws	-2.64		Crippen Method
logp	2.435		Crippen Method
mcvol	162.550	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=C947820&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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