2-Pyrazoline-5-one, 4,4-dimethyl-3-isopropyl-1-phenyl-

Inchi: InChI=1S/C14H18N2O/c1-10(2)12-14(3,4)13(17)16(15-12)11-8-6-5-7-9-11/h5-10H,1-4H3

InchiKey: OTFORNMJURLTPW-UHFFFAOYSA-N

Formula: C14H18N2O

SMILES: CC(C)C1=NN(c2ccccc2)C(=O)C1(C)C

Mol. weight [g/mol]: 230.31

CAS: 92292-40-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.23		Crippen Method
logp	3.071		Crippen Method
mcvol	190.730	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=C92292405&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume