3-tert-Butyl-1-phenyl-2-pyrazolin-5-one

Other names:	3H-Pyrazol-3-one, 5-(1,1-dimethylethyl)-2,4-dihydro-2-phenyl- 2-Pyrazolin-5-one, 3-tert-butyl-1-phenyl-
Inchi:	InChI=1S/C13H16N2O/c1-13(2,3)11-9-12(16)15(14-11)10-7-5-4-6-8-10/h4-8H,9H2,1-3H3
InchiKey:	NOSULZKBEJXMKJ-UHFFFAOYSA-N
Formula:	C13H16N2O
SMILES:	CC(C)(C)C1=NN(c2ccccc2)C(=O)C1
Mol. weight [g/mol]:	216.28
CAS:	6631-89-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	2.825		Crippen Method
mcvol	176.640	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6631896&Units=SI
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

Legend

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

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