

# 3-Pyrazolin-5-one, 4-butyl-1,2-diphenyl-3-methoxy-

Other names:

4-Butyl-1,2-diphenyl-3-methoxy-3-pyrazolin-5-one  
3-Methoxy-4-n-butyl-1,2-diphenyl-5-pyrazolone  
3H-Pyrazol-3-one, 4-butyl-1,2-dihydro-5-methoxy-1,2-diphenyl-  
4-Butyl-5-methoxy-1,2-diphenyl-1,2-dihydro-3H-pyrazol-3-one  
Phenyl butazone, methyl deriv.  
Phenylbutazone, methylated

**Inchi:** InChI=1S/C20H22N2O2/c1-3-4-15-18-19(23)21(16-11-7-5-8-12-16)22(20(18)24-2)17-13

**InchiKey:** HZWCYMHYZRAXMH-UHFFFAOYSA-N

**Formula:** C20H22N2O2

**SMILES:** CCCCc1c(OC)n(-c2ccccc2)n(-c2ccccc2)c1=O

**Mol. weight [g/mol]:** 322.40

**CAS:** 27258-01-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.96		Crippen Method
logp	3.979		Crippen Method
mcvol	257.380	ml/mol	McGowan Method
rinpol	2290.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C27258011&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rinpol:** Non-polar retention indices

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