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/ci990307l

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=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