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

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