Phenylbutazone di-methyl derivative (peak 2)

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]:	322.41

Physical Properties

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

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27258011&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

rinpol: Non-polar retention indices