Oxphenbutazone di-methyl derivative

Other names:	Oxyphenbutazone, dimethyl deriv. Phenylbutazone, hydroxy, bis-methylated 3H-Pyrazol-3-one, 4-butyl-1,2-dihydro-5-methoxy-1-(4-methoxyphenyl)-2-phenyl-
Inchi:	InChI=1S/C21H24N2O3/c1-4-5-11-19-20(24)22(16-9-7-6-8-10-16)23(21(19)26-3)17-12-1
InchiKey:	BAMWJBYBAKIYSU-UHFFFAOYSA-N
Formula:	C21H24N2O3
SMILES:	CCCCc1c(OC)n(-c2ccc(OC)cc2)n(-c2ccccc2)c1=O
Mol. weight [g/mol]:	352.43
CAS:	27383-21-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.08		Crippen Method
logp	3.988		Crippen Method
mcvol	277.340	ml/mol	McGowan Method
rinpol	2500.00		NIST Webbook
rinpol	2500.00		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=C27383217&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