

# Oxphenbutazone di-methyl derivative

<b>Other names:</b>	Oxyphenbutazone, dimethyl deriv. Phenylbutazone, hydroxy, bis-methylated 3H-Pyrazol-3-one, 4-butyl-1,2-dihydro-5-methoxy-1-(4-methoxyphenyl)-2-phenyl-
<b>Inchi:</b>	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
<b>InchiKey:</b>	BAMWJBYBAKIYSU-UHFFFAOYSA-N
<b>Formula:</b>	C21H24N2O3
<b>SMILES:</b>	CCCCc1c(OC)n(-c2ccc(OC)cc2)n(-c2ccccc2)c1=O
<b>Mol. weight [g/mol]:</b>	352.43
<b>CAS:</b>	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
rinpola	2500.00		NIST Webbook
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## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C27383217&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C27383217&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpola:</b>	Non-polar retention indices

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