

# Phenadoxone

<b>Other names:</b>	3-Heptanone, 6-(4-morpholinyl)-4,4-diphenyl- 3-Heptanone, 6-morpholino-4,4-diphenyl- Phenadoxone 3-Heptanone, 4,4-diphenyl-6-morpholino- 4,4-Diphenyl-6-morpholino-3-heptanone 6-Morpholino-4,4-diphenyl-3-heptanone Heptazone Morphodone
<b>Inchi:</b>	InChI=1S/C23H29NO2/c1-3-22(25)23(20-10-6-4-7-11-20,21-12-8-5-9-13-21)18-19(2)24-
<b>InchiKey:</b>	LOXCOAXRHYDLOW-UHFFFAOYSA-N
<b>Formula:</b>	C23H29NO2
<b>SMILES:</b>	<chem>CCC(=O)C(CC(C)N1CCOCC1)(c1ccccc1)c1ccccc1</chem>
<b>Mol. weight [g/mol]:</b>	351.48
<b>CAS:</b>	467-84-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.38		Crippen Method
logp	4.063		Crippen Method
mcvol	293.970	ml/mol	McGowan Method
rinpol	2510.00		NIST Webbook
rinpol	2522.00		NIST Webbook

## Sources

<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=C467845&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C467845&amp;Units=SI</a>
<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>

# 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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