

# 2-Pyrrolidinone, 1-ethyl-4-[2-(4-morpholinyl)ethyl]-3,3-diphenyl-

**Other names:** 2-Pyrrolidinone, 1-ethyl-4-(2-morpholinoethyl)-3,3-diphenyl-

Doxapram

AHR-619

Dopram

1-Ethyl-4-(2-morpholinoethyl)-3,3-diphenyl-2-pyrrolidinone

**Inchi:** InChI=1S/C24H30N2O2/c1-2-26-19-22(13-14-25-15-17-28-18-16-25)24(23(26)27,20-9-5

**InchiKey:** XFDJYSQDBULQSI-UHFFFAOYSA-N

**Formula:** C24H30N2O2

**SMILES:** CCN1CC(CCN2CCOCC2)C(c2ccccc2)(c2ccccc2)C1=O

**Mol. weight [g/mol]:** 378.51

**CAS:** 309-29-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.40		Crippen Method
logp	3.173		Crippen Method
mcvol	307.180	ml/mol	McGowan Method
rinpol	2874.00		NIST Webbook
rinpol	2874.00		NIST Webbook
rinpol	2890.00		NIST Webbook
rinpol	2906.00		NIST Webbook
rinpol	2890.00		NIST Webbook
rinpol	2860.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C309295&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

**Crippen Method:** [https://www.chemed.com/doc/models/crippen\\_log10ws](https://www.chemed.com/doc/models/crippen_log10ws)

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

# 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>rinpol:</b>	Non-polar retention indices

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