

# Buflomedil

<b>Other names:</b>	1-Butanone, 4-(1-pyrrolidinyl)-1-(2,4,6-trimethoxyphenyl)- 2',4',6'-Trimethoxy-4-(1-pyrrolidinyl)butyrophenone
<b>Inchi:</b>	InChI=1S/C17H25NO4/c1-20-13-11-15(21-2)17(16(12-13)22-3)14(19)7-6-10-18-8-4-5-9-
<b>InchiKey:</b>	OWYLAEYXIQKAOL-UHFFFAOYSA-N
<b>Formula:</b>	C17H25NO4
<b>SMILES:</b>	COc1cc(OC)c(C(=O)CCCN2CCCC2)c(OC)c1
<b>Mol. weight [g/mol]:</b>	307.38
<b>CAS:</b>	55837-25-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.47		Crippen Method
logp	2.771		Crippen Method
mcvol	244.930	ml/mol	McGowan Method
rinpol	2388.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C55837257&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55837257&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

## 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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