Buflomedil

Other names:	1-Butanone, 4-(1-pyrrolidinyl)-1-(2,4,6-trimethoxyphenyl)- 2',4',6'-Trimethoxy-4-(1-pyrrolidinyl)butyrophenone
Inchi:	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-
InchiKey:	OWYLAEYXIQKAOL-UHFFFAOYSA-N
Formula:	C17H25NO4
SMILES:	COc1cc(OC)c(C(=O)CCCN2CCCC2)c(OC)c1
Mol. weight [g/mol]:	307.38
CAS:	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

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=C55837257&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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