Zipeprol

Other names: 1-Piperazineethanol, 4-(2-methoxy-2-phenylethyl)-«alpha»-(methoxyphenylmethyl)-«alpha»-(«alpha»-Methoxybenzyl)-4-(«beta»-methoxyphenethyl)-1-piperazineethanol
1-(2-Methoxy-2-phenylethyl)-4-(2-hydroxy-3-methoxy-3-phenylpropyl)piperazine
4-(2-Methoxy-2-phenylethyl)-«alpha»-(methoxyphenylmethyl)-1-piperazineethanol

Inchi: InChI=1S/C23H32N2O3/c1-27-22(19-9-5-3-6-10-19)18-25-15-13-24(14-16-25)17-21(26)2

InchiKey: VSTNNAYSCJQCQI-UHFFFAOYSA-N

Formula: C23H32N2O3

SMILES: COC(CN1CCN(CC(O)C(OC)c2ccccc2)CC1)c1ccccc1

Mol. weight [g/mol]: 384.51

CAS: 34758-83-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	2.740		Crippen Method
mcvol	314.120	ml/mol	McGowan Method
rinpol	2799.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C34758833&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices