

Lobeline

Other names:

Ethanone, 2-[6-(2-hydroxy-2-phenylethyl)-1-methyl-2-piperidinyl]-1-phenyl-,
[2R-[2«alpha»,6«alpha»(S*)]]-
8,10-Diphenyllobellinone

2-(6-(«beta»-Hydroxy-phenethyl)-1-methyl-2-piperidyl)acetophenone

2-(6-(2-Hydroxy-2-phenylethyl)-1-methyl-2-piperidinyl)-1-phenylethanone

Inflatine

Lobelin

«alpha»-Lobeline

Lobnico

(-)-Lobeline

Inchi: InChI=1S/C22H27NO2/c1-23-19(15-21(24)17-9-4-2-5-10-17)13-8-14-20(23)16-22(25)18

InchiKey: MXYUKLILVYORSK-UHFFFAOYSA-N

Formula: C22H27NO2

SMILES: CN1C(CC(=O)c2ccccc2)CCCC1CC(O)c1ccccc1

Mol. weight [g/mol]: 337.46

CAS: 90-69-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.51		Crippen Method
logp	4.236		Crippen Method
mvol	279.880	ml/mol	McGowan Method

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C90697&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/96-178-9/Lobeline.pdf>

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