

Benzoic acid, p-(cyclohexyloxy)-, 3-(2-methylpiperidino)propyl ester

Other names: Benzoic acid, 4-(cyclohexyloxy)-, 3-(2-methyl-1-piperidinyl)propyl ester

Cainasurfa

Cyclocaine

Surfacaine

Surfathesin

Topocaine

Cyclomethycaine

3-(2-Methylpiperidino)propyl p-(cyclohexyloxy)benzoate

Inchi:

InChI=1S/C22H33NO3/c1-18-8-5-6-15-23(18)16-7-17-25-22(24)19-11-13-21(14-12-19)20

InchiKey:

YLRNESBGEGGQBK-UHFFFAOYSA-N

Formula:

C22H33NO3

SMILES:

CC1CCCCN1CCOC(=O)c1ccc(OC2CCCCC2)cc1

Mol. weight [g/mol]:

359.50

CAS:

139-62-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.86		Crippen Method
logp	4.819		Crippen Method
mvol	298.650	ml/mol	McGowan Method

Sources

Crippen Method:

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

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=C139628&Units=SI>

Legend

log10ws:

Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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