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)26

InchiKey: YLRNESBGEGGQBK-UHFFFAOYSA-N

Formula: C22H33NO3

SMILES: CC1CCCCN1CCCOC(=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
mcvol	298.650	ml/mol	McGowan Method

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=C139628&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume