

Cloperastine

Other names:

Piperidine, 1-[2-[(4-chlorophenyl)phenylmethoxy]ethyl]-
Piperidine, 1-(2-((p-chloro-«alpha»-phenylbenzyl)oxy)ethyl)-
1-(2-[(p-Chloro-«alpha»-phenylbenzyl)oxy]ethyl)piperidine

Inchi:

InChI=1S/C20H24ClNO/c21-19-11-9-18(10-12-19)20(17-7-3-1-4-8-17)23-16-15-22-13-5-

InchiKey:

FLNXBVJLPJNOSI-UHFFFAOYSA-N

Formula:

C₂₀H₂₄ClNO

SMILES:

Clc1ccc(C(OCCN2CCCCC2)c2ccccc2)cc1

Mol. weight [g/mol]:

329.86

CAS:

3703-76-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.20		Crippen Method
logp	4.932		Crippen Method
mcvol	262.370	ml/mol	McGowan Method
rropol	2402.00		NIST Webbook

Sources

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3703762&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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
rropol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/11-689-5/Cloperastine.pdf>

Generated by Cheméo on 2024-04-26 20:16:38.711038925 +0000 UTC m=+16451847.631616237.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.