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]: 329.87

Physical Properties

Property code	Value	Unit	Source
logp	4.932		Crippen Method
mcvol	262.370	ml/mol	McGowan Method
rinpol	2402.00		NIST Webbook
tb	659.52	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3703762&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature