

8-Methyl-8-azabicyclo[3.2.1]octan-3-yl 3-chlorobenzoate

Inchi: InChI=1S/C15H18ClNO2/c1-17-12-5-6-13(17)9-14(8-12)19-15(18)10-3-2-4-11(16)7-10/h
InchiKey: UFYVJVZKHDCQOH-UHFFFAOYSA-N
Formula: C15H18ClNO2
SMILES: CN1C2CCC1CC(OC(=O)c1cccc(Cl)c1)C2
Mol. weight [g/mol]: 279.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.02		Crippen Method
logp	3.122		Crippen Method
mcvol	206.390	ml/mol	McGowan Method
rinpol	2172.00		NIST Webbook
rinpol	2172.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U373626&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/43-947-3/8-Methyl-8-azabicyclo-3-2-1-octan-3-yl-3-chlorobenzoate.pdf>

Generated by Cheméo on 2024-04-30 15:59:14.834655797 +0000 UTC m=+16782003.755233117.

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