Metofoline

Inchi: InChI=1S/C20H24ClNO2/c1-22-11-10-15-12-19(23-2)20(24-3)13-17(15)18(22)9-6-14-4-7
InchiKey: YBCPYHQFUMNOJG-UHFFFAOYSA-N
Formula: C20H24ClNO2
SMILES: COc1cc2c(cc1OC)C(CCc1ccc(Cl)cc1)N(C)CC2
Mol. weight [g/mol]: 345.86
CAS: 2154-02-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.38		Crippen Method
logp	4.519		Crippen Method
mcvol	268.240	ml/mol	McGowan Method
rinpol	2635.00		NIST Webbook
rinpol	2635.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2154021&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
rinpol: Non-polar retention indices