

Amoxapine, 7-hydroxy

Inchi: InChI=1S/C17H16ClN3O2/c18-11-1-4-15-13(9-11)17(21-7-5-19-6-8-21)20-14-3-2-12(22)
InchiKey: MEUGUMOVYNSGEW-UHFFFAOYSA-N
Formula: C17H16ClN3O2
SMILES: Oc1ccc2c(c1)Oc1ccc(Cl)cc1C(N1CCNCC1)=N2
Mol. weight [g/mol]: 329.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.27		Crippen Method
logp	3.135		Crippen Method
mcvol	230.770	ml/mol	McGowan Method
rinpol	2900.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R596037&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

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