

Amoxapine

Other names:	Dibenz[b,f][1,4]oxazepine, 2-chloro-11-(1-piperaziny)- Ascendin Asendin 2-Chloro-11-(1-piperaziny)dibenz(b,f)(1,4)oxazepine CL 67772 Demolox Asendis Moxadil Amoxan Amoxepine CL-67.772 2-Chloro-11-(1-piperaziny)dibenzo[b,f][1,4]oxazepine
Inchi:	InChI=1S/C17H16ClN3O/c18-12-5-6-15-13(11-12)17(21-9-7-19-8-10-21)20-14-3-1-2-4-1
InchiKey:	QWGDMFLQWFTERH-UHFFFAOYSA-N
Formula:	C17H16ClN3O
SMILES:	Clc1ccc2c(c1)C(N1CCNCC1)=Nc1cccc1O2
Mol. weight [g/mol]:	313.78
CAS:	14028-44-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.73		Crippen Method
logp	3.429		Crippen Method
mcvol	224.900	ml/mol	McGowan Method
rinpol	2637.00		NIST Webbook
rinpol	2600.00		NIST Webbook
rinpol	2600.00		NIST Webbook
rinpol	2646.00		NIST Webbook
rinpol	2637.00		NIST Webbook
rinpol	2646.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C14028445&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpolar: Non-polar retention indices

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<https://www.chemeo.com/cid/112-562-3/Amoxapine.pdf>

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