Carbinoxamine

Other names: Ethanamine, 2-[(4-chlorophenyl)-2-pyridinylmethoxy]-N,N-dimethyl-
Pyridine, 2-[p-chloro-«alpha»-[2-(dimethylamino)ethoxy]benzyl]-
Allergefon
McN-R 73Z
Paracarbinoxamine
2-(p-Chloro-«alpha»-(2-(dimethylamino)ethoxy)benzyl)pyridine
Paracarinoxamine
Carbinoxamine base
(.+/-.)-Carbinoxamine

Inchi: InChI=1S/C16H19ClN2O/c1-19(2)11-12-20-16(15-5-3-4-10-18-15)13-6-8-14(17)9-7-13/h

InchiKey: OJFSXZCBGQGRNV-UHFFFAOYSA-N

Formula: C16H19ClN2O

SMILES: CN(C)CCOC(c1ccc(Cl)cc1)c1ccccn1

Mol. weight [g/mol]: 290.79

CAS: 486-16-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	3.403		Crippen Method
mcvol	226.850	ml/mol	McGowan Method
rinpol	2047.00		NIST Webbook
rinpol	2109.00		NIST Webbook
rinpol	2067.00		NIST Webbook
rinpol	2060.00		NIST Webbook
rinpol	2052.00		NIST Webbook
rinpol	2047.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2075.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2060.00		NIST Webbook
ripol	2903.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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=C486168&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
ripol:	Polar retention indices