

Zoxazolamine

Other names:	2-Benzoxazolamine, 5-chloro-Benzoxazole, 2-amino-5-chloro-Flexin McN-485 2-Amino-5-chlorobenzoxazole Contrazone USAF MA-12 5-Chloro-2-benzoxazolamine Deflexol Flexilon Zoxamin Zoxine 5-Chlorobenzoxazol-2-ylamine NSC 24995
Inchi:	InChI=1S/C7H5ClN2O/c8-4-1-2-6-5(3-4)10-7(9)11-6/h1-3H,(H2,9,10)
InchiKey:	YGCODSQDUUUKIV-UHFFFAOYSA-N
Formula:	C7H5ClN2O
SMILES:	<chem>Nc1nc2cc(Cl)ccc2o1</chem>
Mol. weight [g/mol]:	168.58
CAS:	61-80-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.09		Crippen Method
logp	2.063		Crippen Method
mccvol	108.640	ml/mol	McGowan Method
rinpol	1629.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61803&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
rinpol:	Non-polar retention indices

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