

Chlorzoxazone

Other names:	2(3H)-Benzoxazolone, 5-chloro- 2-Benzoxazolinone, 5-chloro- 2-Hydroxy-5-chlorobenzoxazole 5-Chlorbenzoxazolin-2-on 5-Chloro-2-benzoxazolinone 5-Chloro-2-benzoxazolol 5-Chloro-2-benzoxazolone 5-Chloro-2-hydroxybenzoxazole 5-Chloro-3(H)-2-benzoxazolone 5-Chlorobenzoksazolinon-2 5-Chlorobenzoksazolon-2 5-Chlorobenzoxazol-2-one 5-Chlorobenzoxazolidone 5-Chlorobenzoxazolinone 5-Chlorobenzoxazolone Biomioran Chloroxazone Chlorzoxazon Escoflex Flexazone Mioran Miotran Myoflexin Myoflexine NSC 26189 Neoflex Paraflex Parafon Forte DSC Pathorysin Solaxin USAF MA-10
Inchi:	InChI=1S/C7H4ClNO2/c8-4-1-2-6-5(3-4)9-7(10)11-6/h1-3H,(H,9,10)
InchiKey:	TZFWZDFKRBELIQ-UHFFFAOYSA-N
Formula:	C7H4ClNO2
SMILES:	O=c1[nH]c2cc(Cl)ccc2o1
Mol. weight [g/mol]:	169.56
CAS:	95-25-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.83		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-2.66		Aqueous Solubility Prediction Method
log10ws	-2.83		Estimated Solubility Method
logp	1.293		Crippen Method
mcvol	104.530	ml/mol	McGowan Method
rinpol	1714.00		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	1728.00		NIST Webbook
tf	366.27	K	Aqueous Solubility Prediction Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95250&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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