

2,1-Benzisoxazole, 5-chloro-3-phenyl-

Other names:	5-Chloro-3-phenylanthranil 5-Chloro-3-phenyl-2,1-benzisoxazole 3-Phenyl-5-chloroanthranil 5-Chloro-3-phenylbenzo[c]isoxazole
Inchi:	InChI=1S/C13H8ClNO/c14-10-6-7-12-11(8-10)13(16-15-12)9-4-2-1-3-5-9/h1-8H
InchiKey:	MUHJZJKVEQASGY-UHFFFAOYSA-N
Formula:	C13H8ClNO
SMILES:	Clc1ccc2noc(-c3ccccc3)c2c1
Mol. weight [g/mol]:	229.66
CAS:	719-64-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.06		Crippen Method
logp	4.148		Crippen Method
mcvol	159.440	ml/mol	McGowan Method

Sources

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=C719642&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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