

2-(P-chlorophenyl)-1(2h)-phthalazone

Inchi:	InChI=1S/C14H9ClN2O/c15-11-5-7-12(8-6-11)17-14(18)13-4-2-1-3-10(13)9-16-17/h1-9H
InchiKey:	QQJQSWFPMBORPH-UHFFFAOYSA-N
Formula:	C14H9ClN2O
SMILES:	O=c1c2ccccc2cnn1-c1ccc(Cl)cc1
Mol. weight [g/mol]:	256.69
CAS:	161716-23-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.80		Crippen Method
logp	3.039		Crippen Method
mcvol	179.210	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C161716230&Units=SI

Legend

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

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<https://www.chemeo.com/cid/117-823-8/2-P-chlorophenyl-1-2h-phthalazone.pdf>

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