

Mecloqualone

Other names:

4(3H)-Quinazolinone, 3-(2-chlorophenyl)-2-methyl-
B 208-Tropon
Casfen
Mecloqualon
Nubarene
4(3H)-Quinazolinone, 3-(o-chlorophenyl)-2-methyl-
W 4744
3-(2-Chlorophenyl)-2-methyl-4(3H)-quinazolinone
CHI 8
2-Methyl-3-(o-chlorophenyl)-4-quinazolinone
2-Methyl-3-(2-chlorophenyl)chinazolon-4
3-(o-Chlorophenyl)-2-methyl-4(3H)-quinazolinone
3-(o-Chlorophenyl)-2-methyl-4-quinazolone
B 208
NSC 142005
2-Methyl-3-(o-chlorophenyl)-4-quinazolone

Inchi:

InChI=1S/C15H11ClN2O/c1-10-17-13-8-4-2-6-11(13)15(19)18(10)14-9-5-3-7-12(14)16/h

InchiKey:

SFITWQDBYUMAPS-UHFFFAOYSA-N

Formula:

C15H11ClN2O

SMILES:

Cc1nc2ccccc2c(=O)n1-c1cccc1Cl

Mol. weight [g/mol]:

270.71

CAS:

340-57-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.28		Crippen Method
logp	3.348		Crippen Method
mcvol	193.300	ml/mol	McGowan Method
rinpole	2255.00		NIST Webbook
rinpole	2255.00		NIST Webbook

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=C340578&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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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