

4-Isoxazolecarboxylic acid, 3-(o-chlorophenyl)-5-methyl-

Other names: 3-(2-chlorophenyl)-5-methylisoxazole-4-carboxylic acid

Inchi: InChI=1S/C11H8ClNO3/c1-6-9(11(14)15)10(13-16-6)7-4-2-3-5-8(7)12/h2-5H,1H3,(H,14,15)

InchiKey: UVEPOHNXGXVOJE-UHFFFAOYSA-N

Formula: C₁₁H₈ClNO₃

SMILES: Cc1onc(-c2ccccc2Cl)c1C(=O)O

Mol. weight [g/mol]: 237.64

CAS: 23598-72-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.80		Crippen Method
logp	3.002		Crippen Method
mcvol	158.160	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C23598723&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

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