2-(4-Chlorophenyl)-5-methoxy-1,3,4-oxadiazole

Inchi: InChI=1S/C9H7ClN2O2/c1-13-9-12-11-8(14-9)6-2-4-7(10)5-3-6/h2-5H,1H3
InchiKey: ZFMXLEKTIPSDTG-UHFFFAOYSA-N
Formula: C9H7ClN2O2
SMILES: COc1nnc(-c2ccc(Cl)cc2)o1
Mol. weight [g/mol]: 210.62
CAS: 82476-12-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.14		Crippen Method
logp	2.399		Crippen Method
mcvol	138.390	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=C82476128&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