

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/ci9903071
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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