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

Inchi: InChI=1S/C10H7N3O2/c1-14-10-13-12-9(15-10)8-4-2-7(6-11)3-5-8/h2-5H,1H3
InchiKey: PVLIPXBIWKNRFI-UHFFFAOYSA-N
Formula: C10H7N3O2
SMILES: COc1nnc(-c2ccc(C#N)cc2)o1
Mol. weight [g/mol]: 201.18
CAS: 109684-94-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.81		Crippen Method
logp	1.617		Crippen Method
mcvol	141.620	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C109684948&Units=SI

Legend

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