Phenol, o-(5-phenyl-1,3,4-oxadiazol-2-yl)-

Inchi: InChI=1S/C14H10N2O2/c17-12-9-5-4-8-11(12)14-16-15-13(18-14)10-6-2-1-3-7-10/h1-9,1

InchiKey: AXKJOWVRUHGNBD-UHFFFAOYSA-N

Formula: C14H10N2O2

SMILES: Oc1ccccc1-c1nnc(-c2ccccc2)o1

Mol. weight [g/mol]: 238.24

CAS: 18233-24-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.49		Crippen Method
logp	3.109		Crippen Method
mcvol	172.840	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18233244&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume