

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,
InchiKey: AXKJOWVRUHGND-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/ci9903071>
Crippen Method: https://www.cheméo.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

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