

2-(4-Bromophenyl)-5-phenyl-1,3,4-oxadiazole

Other names:	1,3,4-Oxadiazole, 2-(4-bromophenyl)-5-phenyl-
Inchi:	InChI=1S/C14H9BrN2O/c15-12-8-6-11(7-9-12)14-17-16-13(18-14)10-4-2-1-3-5-10/h1-9H
InchiKey:	CNLVYZSUMYQALH-UHFFFAOYSA-N
Formula:	C14H9BrN2O
SMILES:	<chem>Brc1ccc(-c2nnc(-c3ccccc3)o2)cc1</chem>
Mol. weight [g/mol]:	301.14
CAS:	21510-43-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.11		Crippen Method
logp	4.166		Crippen Method
mcvol	184.470	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C21510430&Units=SI

Legend

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

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