

2,5-Bis(4-biphenyl)oxazole

Other names:	Oxazole, 2,5-bis([1,1'-biphenyl]-4-yl)- 2,5-di(biphenyl-4-yl)oxazole 2,5-bis(1,1'-biphenyl)oxazole
Inchi:	InChI=1S/C27H19NO/c1-3-7-20(8-4-1)22-11-15-24(16-12-22)26-19-28-27(29-26)25-17-1
InchiKey:	DDZJGFHXUOWOSL-UHFFFAOYSA-N
Formula:	C27H19NO
SMILES:	<chem>c1ccc(-c2ccc(-c3cnc(-c4ccc(-c5ccccc5)cc4)o3)cc2)cc1</chem>
Mol. weight [g/mol]:	373.45
CAS:	2083-09-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-15.38		Crippen Method
logp	7.343		Crippen Method
mcvol	292.640	ml/mol	McGowan Method

Sources

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=C2083092&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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<https://www.chemeo.com/cid/86-495-8/2-5-Bis-4-biphenyl-oxazole.pdf>

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