2-(t-Butylphenyl)-5-(4-biphenylyl)-1,3,4-oxadiazole

Other names:	2-(4-tert-Butylphenyl)-5-(4-biphenyl)-1,3,4-oxadiazole 2-(4-tert-Butylphenyl)-5-(4-biphenylyl)-1,3,4,-oxadiazole 1,3,4-Oxadiazole, 2-[1,1'-biphenyl]-4-yl-5-[4-(1,1-dimethylethyl)phenyl]- Butyl-PBD 1,3,4-Oxadiazole, 2-(4-biphenylyl)-5-(p-tert-butylphenyl)- 2-(4-biphenylyl)-5-(4-tert-butylphenyl)-1,3,4-oxadiazole
Inchi:	InChI=1S/C24H22N2O/c1-24(2,3)21-15-13-20(14-16-21)23-26-25-22(27-23)19-11-9-18(1
InchiKey:	XZCJVWCMJYNSQO-UHFFFAOYSA-N
Formula:	C24H22N2O
SMILES:	CC(C)(C)c1ccc(-c2nnc(-c3ccc(-c4ccccc4)cc3)o2)cc1
Mol. weight [g/mol]:	354.44
CAS:	15082-28-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.86		Crippen Method
logp	6.368		Crippen Method
mcvol	284.110	ml/mol	McGowan Method
rinpol	3342.00		NIST Webbook

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=C15082287&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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