

2,5-Bis(p-(dimethylamino)phenyl)-1,3,4-oxadiazole

Inchi:	InChI=1S/C18H20N4O/c1-21(2)15-9-5-13(6-10-15)17-19-20-18(23-17)14-7-11-16(12-8-1
InchiKey:	FAPXNOXKLZJBMT-UHFFFAOYSA-N
Formula:	C18H20N4O
SMILES:	CN(C)c1ccc(-c2nnc(-c3ccc(N(C)C)cc3)o2)cc1
Mol. weight [g/mol]:	308.38
CAS:	32444-53-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.76		Crippen Method
logp	3.536		Crippen Method
mcvol	243.290	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=C32444534&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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