2,5-di-(3-Methoxyphenyl)-1,3,4-oxadiazole

Other names:	1,3,4-Oxadiazole, 2,5-bis(3-methoxyphenyl)- 2,5-bis(3-methoxyphenyl)-1,3,4-oxadiazole
Inchi:	InChI=1S/C16H14N2O3/c1-19-13-7-3-5-11(9-13)15-17-18-16(21-15)12-6-4-8-14(10-12)2
InchiKey:	VTFRIPCUJGVYKU-UHFFFAOYSA-N
Formula:	C16H14N2O3
SMILES:	COc1cccc(-c2nnc(-c3cccc(OC)c3)o2)c1
Mol. weight [g/mol]:	282.29
CAS:	19748-58-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.18		Crippen Method
logp	3.421		Crippen Method
mcvol	206.890	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C19748584&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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