2,5-Bis(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]: 282.30

Physical Properties

Property code	Value	Unit	Source
hf	-24.97	kJ/mol	Cheméo Relay (1.0)
hvap	117.53	kJ/mol	Cheméo Relay (1.0)
ie	8.26	eV	Cheméo Relay (1.0)
log10ws	-5.15		Cheméo Relay (1.0)
logp	3.421		Crippen Method
mcvol	206.890	ml/mol	McGowan Method
tb	672.11	K	Cheméo Relay (1.0)
tc	946.14	K	Cheméo Relay (1.0)
tf	361.73	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19748584&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point