2,5-BIS[4-BIPHENYLYL]OXAZOLE

Other names: Oxazole, 2,5-bis([1,1'-biphenyl]-4-yl)-
2,5-di(biphenyl-4-yl)oxazole
2,5-bis(1,1'-biphenylyl)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: c1ccc(-c2ccc(-c3cnc(-c4ccc(-c5ccccc5)cc4)o3)cc2)cc1
Mol. weight [g/mol]: 373.45

Physical Properties

Property code	Value	Unit	Source
af	0.7065		Cheméo Relay (1.0)
hf	350.16	kJ/mol	Cheméo Relay (1.0)
hvap	158.42	kJ/mol	Cheméo Relay (1.0)
ie	8.21	eV	Cheméo Relay (1.0)
log10ws	-8.84		Cheméo Relay (1.0)
logp	7.343		Crippen Method
mcvol	292.640	ml/mol	McGowan Method
pc	2075.43	kPa	Cheméo Relay (1.0, beta)
tb	806.93	K	Cheméo Relay (1.0)
tc	1141.60	K	Cheméo Relay (1.0)
tf	490.42	K	Cheméo Relay (1.0)
vc	1.100	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2083092&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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af:	Acentric Factor
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume