

1,4-Bis(5-phenyloxazol-2-yl)benzene

Other names:	POPOP Oxazole, 2,2'-(1,4-phenylene)bis[5-phenyl- p-Bis(5-phenyloxazol-2-yl)benzene Oxazole, 2,2'-p-phenylenebis(5-phenyl- 1,4-Bis(2-(5-phenyloxazolyl))benzene 2,2'-p-Phenylenebis(5-phenyloxazole) 2,2'-(1,4-Phenylene)bis(5-phenyl)oxazole
Inchi:	InChI=1S/C24H16N2O2/c1-3-7-17(8-4-1)21-15-25-23(27-21)19-11-13-20(14-12-19)24-20
InchiKey:	MASVCBBIUQRUKL-UHFFFAOYSA-N
Formula:	C24H16N2O2
SMILES:	<chem>c1ccc(-c2cnc(-c3ccc(-c4ncc(-c5ccccc5)o4)cc3)o2)cc1</chem>
Mol. weight [g/mol]:	364.40
CAS:	1806-34-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-18.88		Crippen Method
logp	6.331		Crippen Method
mcvol	270.520	ml/mol	McGowan Method
rinpol	3525.00		NIST Webbook
rinpol	3525.00		NIST Webbook
rinpol	3525.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	140.00	kJ/mol	480.00	NIST Webbook
hsubt	94.40	kJ/mol	640.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1806344&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hsubt:	Enthalpy of sublimation at a given temperature
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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