Oxazole, 2,5-diphenyl-

Other names:	2,5-Diphenyl-1,3-oxazole
	2,5-diphenyloxazole
	DPO
	DPO (scintillator)
	NSC 24856
	PPO
	PPO (scintillator)
	Tritosol
	USAF EK-6775
Inchi:	InChI=1S/C15H11NO/c1-3-7-12(8-4-1)14-11-16-15(17-14)13-9-5-2-6-10-13/h1-11H
InchiKey:	CNRNYORZJGVOSY-UHFFFAOYSA-N
Formula:	C15H11NO
SMILES:	c1ccc(-c2cnc(-c3ccccc3)o2)cc1
Mol. weight [g/mol]:	221.25
CAS:	92-71-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.18		Crippen Method
logp	4.009		Crippen Method
mcvol	171.080	ml/mol	McGowan Method
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook
tb	633.20	K	NIST Webbook
tf	344.23	K	Thermodynamic properties of phase transitions of phenyl derivatives of maleic anhydride and oxazole
tf	345.00 ± 3.00	K	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic properties of phase transitions of phenyl derivatives of maleic anhydride and oxazole:	https://www.doi.org/10.1016/j.jct.2018.12.001
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92717&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point