PHOSPHONIC ACID, DIPHENYL ESTER

Other names:	Diphenoxyphosphine oxide
	Diphenyl hydrogen phosphite
	Diphenyl phosphite
	Diphenyl phosphonate
	Phenyl phosphonate ((PhO)2HPO)
	Phosphorous acid, diphenyl ester
	Doverphos 213
	Weston DPP
	NSC 43786
Inchi:	InChI=1S/C12H11O3P/c13-16(14-11-7-3-1-4-8-11)15-12-9-5-2-6-10-12/h1-10,16H
InchiKey:	OGBPILLJZSJJRC-UHFFFAOYSA-N
Formula:	C12H11O3P
SMILES:	O=[PH](Oc1ccccc1)Oc1ccccc1
Mol. weight [g/mol]:	234.19

Physical Properties

Property code	Value	Unit	Source
af	0.5787		Cheméo Relay (1.0)
hf	-299.60	kJ/mol	Cheméo Relay (1.0)
hvap	86.20	kJ/mol	Cheméo Relay (1.0)
ie	8.70	eV	Cheméo Relay (1.0)
log10ws	-3.13		Cheméo Relay (1.0)
logp	3.534		Crippen Method
mcvol	170.490	ml/mol	McGowan Method
pc	2857.61	kPa	Cheméo Relay (1.0, beta)
tb	601.96	K	Cheméo Relay (1.0)
tc	842.41	K	Cheméo Relay (1.0)
tf	324.21	K	Cheméo Relay (1.0)

Sources

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):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4712554&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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