Isopropylphenyldiphenyl phosphate

Other names:	Isopropylphenyl diphenyl phosphate
	Propylated triphenyl phosphate
	Syn-O-Ad 8480
Inchi:	InChI=1S/C21H21O4P/c1-17(2)20-15-9-10-16-21(20)25-26(22,23-18-11-5-3-6-12-18)24-
InchiKey:	JJXNVYMIYBNZQX-UHFFFAOYSA-N
Formula:	C21H21O4P
SMILES:	CC(C)c1ccccc1OP(=O)(Oc1ccccc1)Oc1ccccc1
Mol. weight [g/mol]:	368.37

Physical Properties

Property code	Value	Unit	Source
ie	8.51	eV	Cheméo Relay (1.0)
log10ws	-6.14		Cheméo Relay (1.0)
logp	6.455		Crippen Method
mcvol	279.410	ml/mol	McGowan Method
pc	1355.52	kPa	Cheméo Relay (1.0, beta)
tb	674.89	K	Cheméo Relay (1.0)
tc	972.61	K	Cheméo Relay (1.0)
tf	331.05	K	Cheméo Relay (1.0)
vc	1.023	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28108998&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):

Legend

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