DIMETHYL PHENYLPHOSPHONATE

Other names:	Phosphonic acid, phenyl-, dimethyl ester
	O,O-Dimethyl benzene phosphonate
Inchi:	InChI=1S/C8H11O3P/c1-10-12(9,11-2)8-6-4-3-5-7-8/h3-7H,1-2H3
InchiKey:	OXDOANYFRLHSML-UHFFFAOYSA-N
Formula:	C8H11O3P
SMILES:	COP(=O)(OC)c1ccccc1
Mol. weight [g/mol]:	186.15

Physical Properties

Property code	Value	Unit	Source
ie	9.45	eV	Cheméo Relay (1.0)
logp	1.798		Crippen Method
mcvol	137.890	ml/mol	McGowan Method
tf	291.15	K	Cheméo Relay (1.0)

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2240417&Units=SI

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point