

Phosphoric acid, dibutyl phenyl ester

Other names:	Dibutyl phenyl phosphate
Inchi:	InChI=1S/C14H23O4P/c1-3-5-12-16-19(15,17-13-6-4-2)18-14-10-8-7-9-11-14/h7-11H,3-
InchiKey:	YICSVBJRVMLQNS-UHFFFAOYSA-N
Formula:	C14H23O4P
SMILES:	CCCCOP(=O)(OCCCC)Oc1ccccc1
Mol. weight [g/mol]:	286.30
CAS:	2528-36-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.96		Crippen Method
logp	4.807		Crippen Method
mcvol	228.300	ml/mol	McGowan Method
rinpol	1889.00		NIST Webbook
rinpol	1889.00		NIST Webbook
ripol	2596.00		NIST Webbook
ripol	2596.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2528361&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

ripol: Polar retention indices

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