

Phosphoric acid, triheptyl ester

Other names:	Triheptyl phosphate
Inchi:	InChI=1S/C21H45O4P/c1-4-7-10-13-16-19-23-26(22,24-20-17-14-11-8-5-2)25-21-18-15-
InchiKey:	GSURLQOINUQIIH-UHFFFAOYSA-N
Formula:	C21H45O4P
SMILES:	CCCCCCCOP(=O)(CCCCCCCC)CCCCCCCC
Mol. weight [g/mol]:	392.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.14		Crippen Method
logp	8.056		Crippen Method
mcvol	350.690	ml/mol	McGowan Method
rinpol	2459.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U309014&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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