

Phosphorous acid, tris(2,2-dimethylpentyl) ester

Inchi:	InChI=1S/C21H45O3P/c1-10-13-19(4,5)16-22-25(23-17-20(6,7)14-11-2)24-18-21(8,9)15
InchiKey:	SIEJAHKUFLOJRE-UHFFFAOYSA-N
Formula:	C21H45O3P
SMILES:	CCCC(C)(C)COP(OCC(C)(C)CCC)OCC(C)(C)CCC
Mol. weight [g/mol]:	376.55
CAS:	116402-22-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.98		Crippen Method
logp	7.742		Crippen Method
mcvol	344.820	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C116402223&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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