

Phosphoric acid, trioctyl ester

Other names:	Trioctyl phosphate tri-n-Octylphosphate Tris(n-octyl) phosphate
Inchi:	InChI=1S/C24H51O4P/c1-4-7-10-13-16-19-22-26-29(25,27-23-20-17-14-11-8-5-2)28-24-
InchiKey:	WVPGXJOLGGFBCR-UHFFFAOYSA-N
Formula:	C24H51O4P
SMILES:	CCCCCCCCOP(=O)(CCCCCCCC)CCCCCCCC
Mol. weight [g/mol]:	434.63
CAS:	1806-54-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.39		Crippen Method
logp	9.226		Crippen Method
mcvol	392.960	ml/mol	McGowan Method
rinpol	2476.00		NIST Webbook
rinpol	2445.00		NIST Webbook
rinpol	2445.00		NIST Webbook
rinpol	2445.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C1806548&Units=SI

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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<https://www.chemeo.com/cid/65-589-7/Phosphoric-acid-trioctyl-ester.pdf>

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