

Di-tridecyl hydrogen phosphate

Other names:	ditridecyl phosphonate
Inchi:	InChI=1S/C26H55O3P/c1-3-5-7-9-11-13-15-17-19-21-23-25-28-30(27)29-26-24-22-20-18
InchiKey:	BDZYUTQMWUWPLZ-UHFFFAOYSA-N
Formula:	C26H55O3P
SMILES:	CCCCCCCCCCCCCO[PH](=O)CCCCCCCCCCCCC
Mol. weight [g/mol]:	446.69
CAS:	36432-46-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.34		Crippen Method
logp	10.031		Crippen Method
mcvol	415.270	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36432469&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

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