

Phosphonic acid, phenyl-, bis(2-ethyl-4-methylpentyl) ester

Inchi:	InChI=1S/C22H39O3P/c1-7-20(14-18(3)4)16-24-26(23,22-12-10-9-11-13-22)25-17-21(8-
InchiKey:	OZZCXXRALYIASB-UHFFFAOYSA-N
Formula:	C22H39O3P
SMILES:	CCC(COP(=O)(OCC(CC)CC(C)C)c1ccccc1)CC(C)C
Mol. weight [g/mol]:	382.52
CAS:	116401-89-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.00		Crippen Method
logp	6.683		Crippen Method
mcvol	335.150	ml/mol	McGowan Method

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=C116401899&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

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