

Phosphoric acid, tris(2,2,4-trimethylpentyl) ester

Inchi:	InChI=1S/C24H51O4P/c1-19(2)13-22(7,8)16-26-29(25,27-17-23(9,10)14-20(3)4)28-18-2
InchiKey:	PJBLUTNJKONFJA-UHFFFAOYSA-N
Formula:	C24H51O4P
SMILES:	CC(C)CC(C)(C)COP(=O)(OCC(C)(C)CC(C)C)OCC(C)(C)CC(C)C
Mol. weight [g/mol]:	434.63
CAS:	29420-78-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.94		Crippen Method
logp	8.361		Crippen Method
mcvol	392.960	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29420788&Units=SI
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

Legend

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

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