

Propanoic acid, 2-(triphenylphosphoranylidene)-, ethyl ester

Other names:

(Carbethoxyethylidene)triphenylphosphorane
1-Carboethoxyethylidenetriphenylphosphorane
(Carbethoxyethylidene)triphenylphosphorane
Ethyl 2-(triphenylphosphoranylidene)propanoate
Ethyl 2-(triphenylphosphoranylidene)propionate
Propionic acid, 2-(triphenylphosphoranylidene)-, ethyl ester
1-(Ethoxycarbonyl)ethylidenetriphenylphosphorane
1-Ethoxycarbonyl-ethyliden-phosphoran

Inchi: InChI=1S/C23H23O2P/c1-3-25-23(24)19(2)26(20-13-7-4-8-14-20,21-15-9-5-10-16-21)22

InchiKey: KZENFXVDPUMQOE-UHFFFAOYSA-N

Formula: C23H23O2P

SMILES: CCOC(=O)C(C)=P(c1ccccc1)(c1ccccc1)c1ccccc1

Mol. weight [g/mol]: 362.40

CAS: 5717-37-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-14.22		Crippen Method
logp	3.736		Crippen Method
mvol	291.550	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=C5717373&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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