

Phosphoric acid, 2-chloro-3-(diethylamino)-1-methyl-3-oxo-1-propene dimethyl ester, (E)-

Other names:

ENT 25,51
ML 97

OR 1191

(E)-Phosphamidon

trans-Phosphamidon

Phosphamidon (isomer)

Inchi: InChI=1S/C10H19ClNO5P/c1-6-12(7-2)10(13)9(11)8(3)17-18(14,15-4)16-5/h6-7H2,1-5H1

InchiKey: RGCLLPNLLBQHPF-CMDGGOBGSA-N

Formula: C10H19ClNO5P

SMILES: CCN(CC)C(=O)C(Cl)=C(C)OP(=O)(OC)OC

Mol. weight [g/mol]: 299.69

CAS: 297-99-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.88		Crippen Method
logp	2.743		Crippen Method
mcvol	215.190	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=C297994&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

Latest version available from:

<https://www.cheméo.com/cid/122-052-8/Phosphoric-acid-2-chloro-3-diethylamino-1-methyl-3-oxo-1-propenyl-dimethyl>

Generated by Cheméo on 2024-05-06 04:26:13.285849437 +0000 UTC m=+17258822.206426748.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.