[3-chloro-4-(diethylamino)-4-oxobut-2-en-2-yl] dimethyl phosphate

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

InchiKey: RGCLLPNLLBQHPF-UHFFFAOYSA-N

Formula: C10H19ClNO5P

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

Mol. weight [g/mol]: 299.69

CAS: 13171-21-6

Physical Properties

Property code	Value	Unit	Source
logp	2.743		Crippen Method
mcvol	215.190	ml/mol	McGowan Method
tf	228.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point

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