

DIMETHYL (2-OXOPROPYL)PHOSPHONATE

Other names:	Dimethyl acetylmethylphosphonate Phosphonic acid, (2-oxopropyl)-, dimethyl ester
Inchi:	InChI=1S/C5H11O4P/c1-5(6)4-10(7,8-2)9-3/h4H2,1-3H3
InchiKey:	UOWIYNWMROWVDG-UHFFFAOYSA-N
Formula:	C5H11O4P
SMILES:	COP(=O)(CC(C)=O)OC
Mol. weight [g/mol]:	166.11

Physical Properties

Property code	Value	Unit	Source
ie	9.91	eV	Cheméo Relay (1.0)
logp	1.061		Crippen Method
mcvol	120.950	ml/mol	McGowan Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4202146&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/98-456-8/DIMETHYL-2-OXOPROPYL-PHOSPHONATE.pdf>

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