TRIMETHYL PHOSPHONOACETATE

Other names:	Acetic acid, (dimethoxyphosphinyl)-, methyl ester
	Methyl (dimethoxyphosphoryl)acetate
	Trimethyl phosphonacetate
Inchi:	InChI=1S/C5H11O5P/c1-8-5(6)4-11(7,9-2)10-3/h4H2,1-3H3
InchiKey:	SIGOIUCRXKUEIG-UHFFFAOYSA-N
Formula:	C5H11O5P
SMILES:	COC(=O)CP(=O)(OC)OC
Mol. weight [g/mol]:	182.11

Physical Properties

Property code	Value	Unit	Source
af	0.5091		Cheméo Relay (1.0)
hf	-925.67	kJ/mol	Cheméo Relay (1.0)
hvap	67.41	kJ/mol	Cheméo Relay (1.0)
ie	10.24	eV	Cheméo Relay (1.0)
log10ws	0.27		Cheméo Relay (1.0)
logp	0.645		Crippen Method
mcvol	126.820	ml/mol	McGowan Method
pc	2837.20	kPa	Cheméo Relay (1.0, beta)
tb	515.22	K	Cheméo Relay (1.0)
tc	660.84	K	Cheméo Relay (1.0)
tf	241.48	K	Cheméo Relay (1.0)
vc	0.472	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5927184&Units=SI
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):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume