DIETHYL CYANOPHOSPHONATE

Other names:	Phosphorocyanidic acid, diethyl ester
	Phosphorocyanidic acid, O,O-diethyl ester
	Diethoxy-phosphoryl cyanide
	Diethylcyanophosphate
	Diethyl cyanophosphophosphonate
	Diethyl phosphorocyanidate
	Diethyl cyanidophosphate
	Diethylphosphoryl cyanide
Inchi:	InChI=1S/C5H10NO3P/c1-3-8-10(7,5-6)9-4-2/h3-4H2,1-2H3
InchiKey:	ZWWWLCMDTZFSOO-UHFFFAOYSA-N
Formula:	C5H10NO3P
SMILES:	CCOP(=O)(C#N)OCC
Mol. weight [g/mol]:	163.11

Physical Properties

Property code	Value	Unit	Source
hvap	59.36	kJ/mol	Cheméo Relay (1.0)
ie	10.81	eV	Cheméo Relay (1.0)
log10ws	-0.50		Cheméo Relay (1.0)
logp	1.734		Crippen Method
mcvol	120.760	ml/mol	McGowan Method
rinpol	1046.00		NIST Webbook
rinpol	1046.00		NIST Webbook
tb	456.76	K	Cheméo Relay (1.0)
tf	241.94	K	Cheméo Relay (1.0)

Sources

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=C2942587&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point