

Diethyl cyanomethylphosphonate

Other names:	Diethylphosphonoacetonitrile Phosphonic acid, (cyanomethyl)-, diethyl ester (Cyanomethyl)diethoxyphosphine oxide Cyanomethanephosphonic acid, diethyl ester Diethyl cyanomethanephosphonate 2-(Diethylphosphonyl)acetonitrile
Inchi:	InChI=1S/C6H12NO3P/c1-3-9-11(8,6-5-7)10-4-2/h3-4,6H2,1-2H3
InchiKey:	KWMBADTWRIGGGG-UHFFFAOYSA-N
Formula:	C6H12NO3P
SMILES:	CCOP(=O)(CC#N)OCC
Mol. weight [g/mol]:	177.14
CAS:	2537-48-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.65		Crippen Method
logp	1.776		Crippen Method
mcvol	134.850	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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2537486&Units=SI

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.chemeo.com/cid/96-805-2/Diethyl-cyanomethylphosphonate.pdf>

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