

Phosphonic acid, bis(1-methylethyl) ester

Other names:	Phosphonic acid, diisopropyl ester Diisopropyl hydrogen phosphite Diisopropyl phosphite Diisopropyl phosphonate Diisopropylphosphine oxide Isopropyl phosphonate ((C ₃ H ₇ O) ₂ HPO) O,O-Diisopropyl phosphonate di-i-Propylphosphite Diisopropyl hydrogen phosphonate Isopropyl phosphonate NSC 82344
Inchi:	InChI=1S/C6H15O3P/c1-5(2)8-10(7)9-6(3)4/h5-6,10H,1-4H3
InchiKey:	BLKXLEPPVDUHY-UHFFFAOYSA-N
Formula:	C ₆ H ₁₅ O ₃ P
SMILES:	CC(C)O[PH](=O)OC(C)C
Mol. weight [g/mol]:	166.16
CAS:	1809-20-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.19		Crippen Method
logp	2.226		Crippen Method
mcvol	133.470	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1809207&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/42-401-9/Phosphonic-acid-bis-1-methylethyl-ester.pdf>

Generated by Cheméo on 2024-04-26 08:00:26.680992103 +0000 UTC m=+16407675.601569418.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.