

Isopropyl methyl methylphosphonate

Inchi: InChI=1S/C5H13O3P/c1-5(2)8-9(4,6)7-3/h5H,1-4H3
InchiKey: GDBDOLDINYFAKS-UHFFFAOYSA-N
Formula: C5H13O3P
SMILES: COP(C)(=O)OC(C)C
Mol. weight [g/mol]: 152.13
CAS: 690-64-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.48		Crippen Method
logp	1.881		Crippen Method
mcvol	119.380	ml/mol	McGowan Method
rinpol	989.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C690642&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/98-449-6/Isopropyl-methyl-methylphosphonate.pdf>

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