

Diisopropyl methanephosphonate

Other names:	DIMP Diisopropyl methylphosphonate Dimp (phosphonate) Methyl-phosphonic acid diisopropyl ester O,O-Diisopropyl methylphosphonate Phosphonic acid, methyl-, O,O-bis-isopropyl ester Phosphonic acid, methyl-, bis(1-methylethyl) ester Phosphonic acid, methyl-, diisopropyl ester bis(1-methylethyl) methylphosphonate
Inchi:	InChI=1S/C7H17O3P/c1-6(2)9-11(5,8)10-7(3)4/h6-7H,1-5H3
InchiKey:	WOAFDHWYKSOANX-UHFFFAOYSA-N
Formula:	C7H17O3P
SMILES:	CC(C)OP(C)(=O)OC(C)C
Mol. weight [g/mol]:	180.18
CAS:	1445-75-6

Physical Properties

Property code	Value	Unit	Source
hvap	57.60	kJ/mol	NIST Webbook
log10ws	-3.42		Crippen Method
logp	2.659		Crippen Method
mcvol	147.560	ml/mol	McGowan Method
rinpol	1066.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1067.00		NIST Webbook
rinpol	1072.70		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1067.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1073.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	62.10	kJ/mol	360.50	NIST Webbook
hvapt	58.90	kJ/mol	360.50	NIST Webbook
hvapt	56.50	kJ/mol	360.50	NIST Webbook
hvapt	54.20	kJ/mol	360.50	NIST Webbook
hvapt	52.40	kJ/mol	360.50	NIST Webbook
pvap	0.81	kPa	341.60	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	1.88e-03	kPa	263.20	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	5.02e-03	kPa	273.20	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	0.01	kPa	283.20	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	0.03	kPa	293.20	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	0.65	kPa	338.90	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	0.67	kPa	339.80	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds

pvap	6.19e-04	kPa	253.20	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	0.81	kPa	342.10	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	1.04	kPa	346.20	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	1.08	kPa	347.00	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	1.35	kPa	350.90	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	2.01	kPa	358.00	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	3.20	kPa	367.40	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	4.68	kPa	376.00	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	7.99	kPa	388.60	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	10.65	kPa	396.10	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds

pvap	19.87	kPa	412.10	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	39.96	kPa	434.40	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	100.30	kPa	468.00	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1445756&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds:	https://www.doi.org/10.1021/je8010024

Legend

hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices

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