

Diethyl methanephosphonate

Other names:	DEMP Diethoxymethylphosphine oxide Methylphosphonic acid, diethyl ester O,O-diethyl methylphosphonate diethyl methylphosphonate phosphonic acid, methyl-, diethyl ester
Inchi:	InChI=1S/C5H13O3P/c1-4-7-9(3,6)8-5-2/h4-5H2,1-3H3
InchiKey:	NYYLZXREFNYPKB-UHFFFAOYSA-N
Formula:	C5H13O3P
SMILES:	CCOP(C)(=O)OCC
Mol. weight [g/mol]:	152.13
CAS:	683-08-9

Physical Properties

Property code	Value	Unit	Source
hvap	55.90	kJ/mol	NIST Webbook
log10ws	-2.36		Crippen Method
logp	1.882		Crippen Method
mcvol	119.380	ml/mol	McGowan Method
rinpol	975.00		NIST Webbook
rinpol	1006.50		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	1006.50		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	1015.10		NIST Webbook
rinpol	1015.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	60.60	kJ/mol	359.00	NIST Webbook
hvapt	57.20	kJ/mol	359.00	NIST Webbook
hvapt	54.70	kJ/mol	359.00	NIST Webbook

hvapt	53.40	kJ/mol	359.00	NIST Webbook
hvapt	51.20	kJ/mol	359.00	NIST Webbook
hvapt	51.80	kJ/mol	372.50	NIST Webbook
pvap	0.28	kPa	324.70	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	2.56e-03	kPa	263.20	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	6.88e-03	kPa	273.20	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	0.02	kPa	283.20	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	0.04	kPa	293.20	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	0.15	kPa	316.80	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	0.19	kPa	318.90	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	0.23	kPa	321.10	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	0.25	kPa	322.20	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds

pvap	8.62e-04	kPa	253.20	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	0.36	kPa	327.30	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	0.47	kPa	331.10	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	0.64	kPa	335.20	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	0.80	kPa	339.80	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	0.96	kPa	343.30	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	1.17	kPa	346.40	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	1.66	kPa	353.30	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	2.36	kPa	359.40	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	4.00	kPa	370.30	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds

pvap	6.64	kPa	382.60	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	12.01	kPa	397.30	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	20.03	kPa	411.00	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	40.05	kPa	433.30	Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds
pvap	101.40	kPa	465.90	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=C683089&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental Determination of the Solubilities of CO₂ and CH₄ in Diethyl Methyl Phosphite:	https://www.doi.org/10.1021/je200237u
Vapor Pressure of Organophosphorus Nerve Agent Simulant Compounds:	https://www.doi.org/10.1021/je8010024

Legend

h_{vap}:	Enthalpy of vaporization at standard conditions
h_{vapt}:	Enthalpy of vaporization at a given temperature
log_{10ws}:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

pvap: Vapor pressure
rinpol: Non-polar retention indices

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