Trimethyl phosphite

Other names:	Methyl phosphite ((MeO)3P)
	NSC 6513
	P(OCH3)3
	Phosphorous acid, trimethyl ester
	Trimethoxyfosfin
	Trimethoxyphosphine
	Trimethyl ester of phosphorous acid
	Trimethylfosfit
	UN 2329
Inchi:	InChI=1S/C3H9O3P/c1-4-7(5-2)6-3/h1-3H3
InchiKey:	CYTQBVOFDCPGCX-UHFFFAOYSA-N
Formula:	C3H9O3P
SMILES:	COP(OC)OC
Mol. weight [g/mol]:	124.08
CAS:	121-45-9

Physical Properties

Property code	Value	Unit	Source
affp	929.70	kJ/mol	NIST Webbook
basg	899.90	kJ/mol	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	9.21	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	9.00 ± 0.05	eV	NIST Webbook
ie	8.92	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.22	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.25	eV	NIST Webbook
log10ws	2.83		Crippen Method
logp	1.153		Crippen Method
mcvol	91.200	ml/mol	McGowan Method
rinpol	689.00		NIST Webbook
rinpol	688.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	176.65	J/mol×K	299.05	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzonitrile, and 2-Dimethylphosphonomethylbenzonitrile
cpl	179.14	J/mol×K	302.10	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzonitrile, and 2-Dimethylphosphonomethylbenzonitrile
cpl	180.68	J/mol×K	305.10	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzonitrile, and 2-Dimethylphosphonomethylbenzonitrile
cpl	183.16	J/mol×K	308.15	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzonitrile, and 2-Dimethylphosphonomethylbenzonitrile
cpl	183.86	J/mol×K	310.95	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzonitrile, and 2-Dimethylphosphonomethylbenzonitrile
cpl	187.75	J/mol×K	313.75	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzonitrile, and 2-Dimethylphosphonomethylbenzonitrile

cpl	188.67	J/mol×K	316.73	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzonitrile, and 2-Dimethylphosphonomethylbenzonitrile
cpl	192.12	J/mol×K	319.69	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzonitrile, and 2-Dimethylphosphonomethylbenzonitrile
cpl	194.20	J/mol×K	322.33	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzonitrile, and 2-Dimethylphosphonomethylbenzonitrile
cpl	195.38	J/mol×K	325.90	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzonitrile, and 2-Dimethylphosphonomethylbenzonitrile
cpl	196.91	J/mol×K	329.00	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzonitrile, and 2-Dimethylphosphonomethylbenzonitrile
cpl	200.37	J/mol×K	331.35	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzonitrile, and 2-Dimethylphosphonomethylbenzonitrile
cpl	202.37	J/mol×K	335.89	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzonitrile, and 2-Dimethylphosphonomethylbenzonitrile

cpl	204.19	J/mol×K	337.70	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzonitrile, and 2-Dimethylphosphonomethylbenzonitrile
cpl	207.44	J/mol×K	340.75	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzonitrile, and 2-Dimethylphosphonomethylbenzonitrile
cpl	212.11	J/mol×K	343.73	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzonitrile, and 2-Dimethylphosphonomethylbenzonitrile
cpl	214.53	J/mol×K	348.05	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzonitrile, and 2-Dimethylphosphonomethylbenzonitrile
hvapt	42.50	kJ/mol	322.00	NIST Webbook
hvapt	32.80	kJ/mol	458.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121459&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzonitrile, and 2-Dimethylphosphonomethylbenzonitrile:	https://www.doi.org/10.1021/je060445o
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
cpl:	Liquid phase heat capacity

hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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