

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	9.40	eV	NIST Webbook
ie	8.40	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	9.25	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.22	eV	NIST Webbook
log10ws	2.83		Crippen Method
logp	1.153		Crippen Method
mcvol	91.200	ml/mol	McGowan Method
rinpol	688.00		NIST Webbook
rinpol	689.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	214.53	J/molxK	348.05	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzotrile, and 2-Dimethylphosphonomethylbenzotrile
cpl	212.11	J/molxK	343.73	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzotrile, and 2-Dimethylphosphonomethylbenzotrile
cpl	176.65	J/molxK	299.05	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzotrile, and 2-Dimethylphosphonomethylbenzotrile
cpl	179.14	J/molxK	302.10	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzotrile, and 2-Dimethylphosphonomethylbenzotrile
cpl	180.68	J/molxK	305.10	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzotrile, and 2-Dimethylphosphonomethylbenzotrile
cpl	183.16	J/molxK	308.15	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzotrile, and 2-Dimethylphosphonomethylbenzotrile

cpl	183.86	J/mol×K	310.95	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzotrile, and 2-Dimethylphosphonomethylbenzotrile
cpl	187.75	J/mol×K	313.75	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzotrile, and 2-Dimethylphosphonomethylbenzotrile
cpl	188.67	J/mol×K	316.73	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzotrile, and 2-Dimethylphosphonomethylbenzotrile
cpl	192.12	J/mol×K	319.69	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzotrile, and 2-Dimethylphosphonomethylbenzotrile
cpl	194.20	J/mol×K	322.33	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzotrile, and 2-Dimethylphosphonomethylbenzotrile
cpl	195.38	J/mol×K	325.90	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzotrile, and 2-Dimethylphosphonomethylbenzotrile
cpl	196.91	J/mol×K	329.00	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzotrile, and 2-Dimethylphosphonomethylbenzotrile

cpl	200.37	J/molxK	331.35	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzotrile, and 2-Dimethylphosphonomethylbenzotrile
cpl	202.37	J/molxK	335.89	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzotrile, and 2-Dimethylphosphonomethylbenzotrile
cpl	204.19	J/molxK	337.70	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzotrile, and 2-Dimethylphosphonomethylbenzotrile
cpl	207.44	J/molxK	340.75	Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzotrile, and 2-Dimethylphosphonomethylbenzotrile
hvapt	32.80	kJ/mol	458.00	NIST Webbook
hvapt	42.50	kJ/mol	322.00	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/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzotrile, and 2-Dimethylphosphonomethylbenzotrile: <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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