Phosphine, triphenyl-

Other names:	NSC 10
	NSC 215203
	PP 360
	Phosphorus triphenyl
	Trifenylfosfin
	Triphenylphosphane
	Triphenylphosphide
	Triphenylphosphine
	Triphenylphosphorus
Inchi:	InChI=1S/C18H15P/c1-4-10-16(11-5-1)19(17-12-6-2-7-13-17)18-14-8-3-9-15-18/h1-15H
InchiKey:	RIOQSEWOXXDEQQ-UHFFFAOYSA-N
Formula:	C18H15P
SMILES:	c1ccc(P(c2ccccc2)c2ccccc2)cc1
Mol. weight [g/mol]:	262.29
CAS:	603-35-0

Physical Properties

Property code	Value	Unit	Source
affp	972.80	kJ/mol	NIST Webbook
basg	940.40	kJ/mol	NIST Webbook
hsub	113.20 ± 3.00	kJ/mol	NIST Webbook
hsub	96.20 ± 8.40	kJ/mol	NIST Webbook
ie	7.85 ± 0.05	eV	NIST Webbook
ie	7.37 ± 0.01	eV	NIST Webbook
ie	7.83	eV	NIST Webbook
ie	8.20 ± 0.05	eV	NIST Webbook
ie	7.36 ± 0.05	eV	NIST Webbook
ie	7.80 ± 0.05	eV	NIST Webbook
ie	7.97	eV	NIST Webbook
ie	7.44 ± 0.05	eV	NIST Webbook
ie	7.92	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
log10ws	-13.68		Crippen Method
logp	3.445		Crippen Method
mcvol	213.660	ml/mol	McGowan Method

tf	352.65	K	Solubilities of Phenylphosphinic Acid, Hydroxymethylphenylphosphinic Acid, p-Methoxyphenylphosphinic Acid, p-Methoxyphenylhydroxymethylphosphini Acid, Triphenylphosphine, Tri(p-methoxyphenyl)phosphine, and Tri(p-methoxyphenyl)phosphine Oxide in Selected Solvents
tf	354.40 ± 0.50	K	NIST Webbook
tf	353.70 ± 0.50	K	NIST Webbook
tf	350.40 ± 1.00	K	NIST Webbook
tf	347.85 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	312.50	J/mol×K	298.50	NIST Webbook
hfust	19.69	kJ/mol	354.40	NIST Webbook
hfust	19.69	kJ/mol	354.40	NIST Webbook
hfust	19.69	kJ/mol	354.40	NIST Webbook
hsubt	109.20 ± 1.10	kJ/mol	350.00	NIST Webbook
hvapt	71.20	kJ/mol	571.50	NIST Webbook
hvapt	91.00 ± 2.00	kJ/mol	378.00	NIST Webbook
sfust	55.56	J/mol×K	354.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57798e+01
Coeff. B	-6.25733e+03
Coeff. C	-8.95290e+01
Temperature range (K), min.	493.15
Temperature range (K), max.	687.15

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermochemistry of adducts of some bivalent transition metal bromides with triphenylphosphine:	https://www.doi.org/10.1016/j.tca.2005.06.016
Solubility Determination and Thermodynamic Modeling of Sodium Thioglycolate in Pure and Binary Solvent Mixtures from 278.15 to 323.15 K:	https://www.doi.org/10.1021/acs.jced.7b00245
Solubilities of Triphenylphosphine in Ethanol, 2-Propanol, Acetone, Benzene, and Styrene:	https://www.doi.org/10.1021/je060350m
Solubilities of Phenylphosphinic Acid, Hydroxymethylphenylphosphinic Acid, p-Methoxyphenylphosphinic Acid, p-Methoxyphenylhydroxymethylphosphinic Acid, Triphenylphosphine, Tri(p-methoxyphenyl)phosphine, and Tri(p-methoxyphenyl)phosphine Oxide in Selected Solvents:	https://www.doi.org/10.1021/je050377q
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C603350&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
cps:	Solid phase heat capacity
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
pvap:	Vapor pressure
sfust:	Entropy of fusion at a given temperature
tf:	Normal melting (fusion) point

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