

Phosphorus pentafluoride

Other names:	PF5 Phosphorane, pentafluoro- Phosphorus fluoride Phosphorus(V) fluoride UN 2198
Inchi:	InChI=1S/F5P/c1-6(2,3,4)5
InchiKey:	OBCUTHMOOONNBS-UHFFFAOYSA-N
Formula:	F5P
SMILES:	FP(F)(F)(F)F
Mol. weight [g/mol]:	125.97
CAS:	7647-19-0

Physical Properties

Property code	Value	Unit	Source
ea	0.75 ± 0.15	eV	NIST Webbook
ie	15.54	eV	NIST Webbook
ie	15.60	eV	NIST Webbook
log10ws	0.99		Crippen Method
logp	2.962		Crippen Method
mcvol	44.470	ml/mol	McGowan Method
tb	188.30	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	17.20	kJ/mol	184.00	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.01246e+01
Coeff. B	-2.63297e+03
Coeff. C	-1.87500e+01
Temperature range (K), min.	116.15
Temperature range (K), max.	188.55

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7647190&Units=SI
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/ci9903071

Legend

ea:	Electron affinity
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
tb:	Normal Boiling Point Temperature

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