Pyridine, pentafluoro-

Other names:	2,3,4,5,6-Pentafluoropyridine
	Pentafluoropyridine
	Perfluoropyridine
Inchi:	InChI=1S/C5F5N/c6-1-2(7)4(9)11-5(10)3(1)8
InchiKey:	XTGOWLIKIQLYRG-UHFFFAOYSA-N
Formula:	C5F5N
SMILES:	Fc1nc(F)c(F)c(F)c1F
Mol. weight [g/mol]:	169.05
CAS:	700-16-3

Physical Properties

Property code	Value	Unit	Source
affp	764.90	kJ/mol	NIST Webbook
basg	733.00	kJ/mol	NIST Webbook
ea	0.68 ± 0.11	eV	NIST Webbook
ea	0.70 ± 0.05	eV	NIST Webbook
ie	10.30	eV	NIST Webbook
ie	10.08	eV	NIST Webbook
ie	10.27	eV	NIST Webbook
ie	10.07	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
log10ws	-2.90		Crippen Method
logp	1.777		Crippen Method
mcvol	76.380	ml/mol	McGowan Method
tb	357.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	36.30	kJ/mol	318.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.68584e+01
Coeff. B	-4.37031e+03
Temperature range (K), min.	263.74
Temperature range (K), max.	378.48

Sources

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
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=C700163&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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