p-Fluoroaniline

Other names:	Benzenamine, 4-fluoro- Aniline, p-fluoro- p-Fluorophenylamine 4-Fluoroaniline 4-Fluoronaniline 4-Fluorobenzenamine Aniline, 4-fluoro- 1-Amino-4-fluorobenzene 4-Fluoranilin UN 2944 NSC 579
Inchi:	InChI=1S/C6H6FN/c7-5-1-3-6(8)4-2-5/h1-4H,8H2
InchiKey:	KRZCOLNOCZKSDF-UHFFFAOYSA-N
Formula:	C6H6FN
SMILES:	Nc1ccc(F)cc1
Mol. weight [g/mol]:	111.12
CAS:	371-40-4

Physical Properties

Property code	Value	Unit	Source
affp	871.50	kJ/mol	NIST Webbook
basg	839.70	kJ/mol	NIST Webbook
chl	-3273.00	kJ/mol	NIST Webbook
gf	-25.94	kJ/mol	Joback Method
hf	-104.43	kJ/mol	Joback Method
hfus	13.22	kJ/mol	Joback Method
hvap	54.80 ± 0.80	kJ/mol	NIST Webbook
ie	8.18	eV	NIST Webbook
ie	8.18	eV	NIST Webbook
ie	7.90 ± 0.10	eV	NIST Webbook
log10ws	-1.44		Crippen Method
logp	1.408		Crippen Method
mcvol	83.390	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
rinpol	967.60		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	967.60		NIST Webbook

rinpol	1001.00		NIST Webbook
rinpol	996.00		NIST Webbook
tb	461.00	K	NIST Webbook
tc	658.85	K	Joback Method
tf	271.25	K	NIST Webbook
tf	314.65 ± 1.50	K	NIST Webbook
vc	0.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.82	J/mol×K	440.14	Joback Method
cpg	167.25	J/mol×K	476.59	Joback Method
cpg	176.10	J/mol×K	513.04	Joback Method
cpg	184.40	J/mol×K	549.50	Joback Method
cpg	192.17	J/mol×K	585.95	Joback Method
cpg	199.43	J/mol×K	622.40	Joback Method
cpg	206.21	J/mol×K	658.85	Joback Method
cpl	195.20	J/mol×K	298.15	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	460.20	K	102.00	NIST Webbook
tbrp	358.20	K	2.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C371404&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume