Benzenamine, 2,3,4,5,6-pentafluoro-

Other names:	Aniline, 2,3,4,5,6-pentafluoro-
	Pentafluoroaniline
	Pentafluorophenylamine
	2,3,4,5,6-Pentafluoroaniline
	Aminopentafluorobenzene
	1-Amino-2,3,4,5,6-pentafluorobenzene
Inchi:	InChI=1S/C6H2F5N/c7-1-2(8)4(10)6(12)5(11)3(1)9/h12H2
InchiKey:	NOXLGCOSAFGMDV-UHFFFAOYSA-N
Formula:	C6H2F5N
SMILES:	Nc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	183.08
CAS:	771-60-8

Physical Properties

Property code	Value	Unit	Source
gf	-843.70	kJ/mol	Joback Method
hf	-934.75	kJ/mol	Joback Method
hfus	23.99	kJ/mol	Joback Method
hvap	41.09	kJ/mol	Joback Method
ie	8.90	eV	NIST Webbook
ie	8.40 ± 0.02	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
log10ws	-2.76		Crippen Method
logp	1.964		Crippen Method
mcvol	90.470	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
ss	246.23	J/mol×K	NIST Webbook
tb	426.70	K	NIST Webbook
tb	426.00	K	NIST Webbook
tc	638.12	K	Joback Method
tf	332.61	K	Joback Method
tt	306.75 ± 0.03	K	NIST Webbook
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.64	J/mol×K	638.12	Joback Method
cpg	219.70	J/mol×K	607.96	Joback Method
cpg	191.58	J/mol×K	457.14	Joback Method
cpg	197.66	J/mol×K	487.30	Joback Method
cpg	203.50	J/mol×K	517.47	Joback Method
cpg	209.13	J/mol×K	547.63	Joback Method
cpg	214.52	J/mol×K	577.80	Joback Method
cps	230.79	J/mol×K	298.15	NIST Webbook
hfust	14.27	kJ/mol	306.80	NIST Webbook
hfust	3.94	kJ/mol	287.40	NIST Webbook
hfust	14.27	kJ/mol	306.80	NIST Webbook
sfust	46.51	J/mol×K	306.80	NIST Webbook
sfust	13.71	J/mol×K	287.40	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C771608&Units=SI

Legend

cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume