Benzene, pentafluoronitro-

Other names:	Nitropentafluorobenzene
	Pentafluoronitrobenzene
	1,2,3,4,5-Pentafluoro-6-nitrobenzene
Inchi:	InChI=1S/C6F5NO2/c7-1-2(8)4(10)6(12(13)14)5(11)3(1)9
InchiKey:	INUOFQAJCYUOJR-UHFFFAOYSA-N
Formula:	C6F5NO2
SMILES:	O=[N+]([O-])c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	213.06
CAS:	880-78-4

Physical Properties

Property code	Value	Unit	Source
ea	1.45 ± 0.11	eV	NIST Webbook
ea	1.50 ± 0.25	eV	NIST Webbook
gf	-874.60	kJ/mol	Joback Method
hf	-979.30	kJ/mol	Joback Method
hfus	30.15	kJ/mol	Joback Method
hvap	47.04	kJ/mol	Joback Method
ie	10.66	eV	NIST Webbook
log10ws	-3.78		Crippen Method
logp	2.290		Crippen Method
mcvol	97.910	ml/mol	McGowan Method
pc	3261.58	kPa	Joback Method
sl	323.13	J/mol×K	NIST Webbook
tb	432.70	K	NIST Webbook
tc	736.58	K	Joback Method
tf	392.96	K	Joback Method
tt	250.50 ± 0.20	K	NIST Webbook
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.73	J/mol×K	569.80	Joback Method

cpg	229.68	J/mol×K	603.16	Joback Method
cpg	235.32	J/mol×K	636.51	Joback Method
cpg	240.64	J/mol×K	669.87	Joback Method
cpg	245.65	J/mol×K	703.22	Joback Method
cpg	217.45	J/mol×K	536.45	Joback Method
cpg	250.35	J/mol×K	736.58	Joback Method
cpl	272.96	J/mol×K	298.15	NIST Webbook
hfust	11.81	kJ/mol	250.50	NIST Webbook
hfust	11.81	kJ/mol	250.50	NIST Webbook
hfust	11.81	kJ/mol	250.50	NIST Webbook
sfust	47.13	J/mol×K	250.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C880784&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

cpg: Ideal gas heat capacity
cpl: Liquid phase heat capacity
ea: Electron affinity
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
sl: Liquid 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