Benzene, 1-fluoro-4-nitro-

Other names:	p-Fluoronitrobenzene
	p-Nitrofluorobenzene
	1-Fluoro-4-nitrobenzene
	1-Nitro-4-fluorobenzene
	1,4-Fluoronitrobenzene
	4-Fluoronitrobenzene
	4-Nitrofluorobenzene
Inchi:	InChI=1S/C6H4FNO2/c7-5-1-3-6(4-2-5)8(9)10/h1-4H
InchiKey:	WFQDTOYDVUWQMS-UHFFFAOYSA-N
Formula:	C6H4FNO2
SMILES:	O=[N+]([O-])c1ccc(F)cc1
Mol. weight [g/mol]:	141.10
CAS:	350-46-9

Physical Properties

Property code	Value	Unit	Source
chs	-2941.10	kJ/mol	NIST Webbook
ea	1.15 ± 0.05	eV	NIST Webbook
ea	1.10 ± 0.05	eV	NIST Webbook
ea	1.08 ± 0.09	eV	NIST Webbook
ea	1.12 ± 0.10	eV	NIST Webbook
gf	-56.84	kJ/mol	Joback Method
hf	-148.98	kJ/mol	Joback Method
hfus	19.39	kJ/mol	Joback Method
hvap	47.66	kJ/mol	Joback Method
ie	10.00 ± 0.10	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
log10ws	-2.45		Crippen Method
logp	1.734		Crippen Method
mcvol	90.830	ml/mol	McGowan Method
pc	4379.97	kPa	Joback Method
tb	478.20	K	NIST Webbook
tb	478.00	K	NIST Webbook
tc	760.95	K	Joback Method
tf	340.52	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.84	J/mol×K	519.45	Joback Method
cpg	197.17	J/mol×K	559.70	Joback Method
cpg	205.79	J/mol×K	599.95	Joback Method
cpg	213.75	J/mol×K	640.20	Joback Method
cpg	221.07	J/mol×K	680.45	Joback Method
cpg	227.79	J/mol×K	720.70	Joback Method
cpg	233.94	J/mol×K	760.95	Joback Method

Sources

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=C350469&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas 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
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
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume