Benzene, 1-fluoro-3-nitro-

Other names:	m-Fluoronitrobenzene
	m-Nitrofluorobenzene
	1-Fluoro-3-nitrobenzene
	3-Fluoronitrobenzene
Inchi:	InChI=1S/C6H4FNO2/c7-5-2-1-3-6(4-5)8(9)10/h1-4H
InchiKey:	WMASLRCNNKMRFP-UHFFFAOYSA-N
Formula:	C6H4FNO2
SMILES:	O=[N+]([O-])c1cccc(F)c1
Mol. weight [g/mol]:	141.10
CAS:	402-67-5

Physical Properties

Property code	Value	Unit	Source
chl	-2955.40	kJ/mol	NIST Webbook
ea	1.24 ± 0.10	eV	NIST Webbook
ea	1.21 ± 0.09	eV	NIST Webbook
ea	1.24 ± 0.05	eV	NIST Webbook
ea	1.21 ± 0.05	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	9.88	eV	NIST Webbook
ie	9.90 ± 0.10	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
rinpol	1067.00		NIST Webbook
rinpol	1067.00		NIST Webbook
tb	473.50 ± 0.50	K	NIST Webbook
tb	478.20	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	359.20	K	2.50	NIST Webbook

Sources

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=C402675&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl: Standard liquid 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
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