

Benzene, 1-fluoro-2-nitro-

Other names:	o-Fluoronitrobenzene o-Nitrofluorobenzene Benzene, o-nitrofluoro- 1-Fluoro-2-nitrobenzene 2-Fluoronitrobenzene 2-Nitrofluorobenzene
Inchi:	InChI=1S/C6H4FNO2/c7-5-3-1-2-4-6(5)8(9)10/h1-4H
InchiKey:	PWKNBLFSJAVFAB-UHFFFAOYSA-N
Formula:	C6H4FNO2
SMILES:	O=[N+](O)c1cccc1F
Mol. weight [g/mol]:	141.10
CAS:	1493-27-2

Physical Properties

Property code	Value	Unit	Source
chl	-2960.00	kJ/mol	NIST Webbook
ea	1.11 ± 0.05	eV	NIST Webbook
ea	1.24 ± 0.05	eV	NIST Webbook
ea	1.08 ± 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	9.86	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	487.50 ± 0.50	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	389.20	K	2.90	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=C1493272&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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