Phenol, 3-fluoro-4-nitro-

Other names: 3-Fluoro-4-nitrophenol
Inchi: InChI=1S/C6H4FNO3/c7-5-3-4(9)1-2-6(5)8(10)11/h1-3,9H
InchiKey: CSSGKHVRDGATJL-UHFFFAOYSA-N
Formula: C6H4FNO3
SMILES: O=[N+]([O-])c1ccc(O)cc1F
Mol. weight [g/mol]: 157.10
CAS: 394-41-2

Physical Properties

Property code	Value	Unit	Source
gf	-211.46	kJ/mol	Joback Method
hf	-326.29	kJ/mol	Joback Method
hfus	25.17	kJ/mol	Joback Method
hvap	60.68	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.439		Crippen Method
mcvol	96.700	ml/mol	McGowan Method
pc	5390.71	kPa	Joback Method
tb	600.07	K	Joback Method
tc	852.64	K	Joback Method
tf	452.24	K	Joback Method
vc	0.330	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.12	J/mol×K	600.07	Joback Method
cpg	234.01	J/mol×K	642.17	Joback Method
cpg	241.21	J/mol×K	684.26	Joback Method
cpg	247.81	J/mol×K	726.36	Joback Method
cpg	253.92	J/mol×K	768.45	Joback Method
cpg	259.63	J/mol×K	810.55	Joback Method
cpg	265.04	J/mol×K	852.64	Joback Method

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=C394412&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
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