Phenol, 3-fluoro-

Other names:	3-FLUOROPHENOL
	3-Fluorphenol
	Phenol, m-fluoro-
	m-Fluorophenol
Inchi:	InChI=1S/C6H5FO/c7-5-2-1-3-6(8)4-5/h1-4,8H
InchiKey:	SJTBRFHBXDZMPS-UHFFFAOYSA-N
Formula:	C6H5FO
SMILES:	Oc1cccc(F)c1
Mol. weight [g/mol]:	112.10
CAS:	372-20-3

Physical Properties

Property code	Value	Unit	Source
affp	802.00	kJ/mol	NIST Webbook
basg	772.00	kJ/mol	NIST Webbook
chl	-2915.00	kJ/mol	NIST Webbook
gf	-237.38	kJ/mol	Joback Method
hf	-304.06	kJ/mol	Joback Method
hfus	14.20	kJ/mol	Joback Method
hvap	60.10 ± 0.90	kJ/mol	NIST Webbook
ie	8.73 ± 0.03	eV	NIST Webbook
ie	8.99	eV	NIST Webbook
ie	9.05 ± 0.02	eV	NIST Webbook
log10ws	-1.35		Crippen Method
logp	1.531		Crippen Method
mcvol	79.280	ml/mol	McGowan Method
pc	5414.53	kPa	Joback Method
tb	451.20	K	NIST Webbook
tb	450.95	K	KDB
tc	663.74	K	Joback Method
tf	286.65	K	KDB
vc	0.247	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	154.19	J/mol×K	443.25	Joback Method
cpg	163.19	J/mol×K	480.00	Joback Method
cpg	171.42	J/mol×K	516.75	Joback Method
cpg	178.95	J/mol×K	553.49	Joback Method
cpg	185.85	J/mol×K	590.24	Joback Method
cpg	192.19	J/mol×K	626.99	Joback Method
cpg	198.03	J/mol×K	663.74	Joback Method
hvapt	60.10	kJ/mol	298.15	Experimental and Computational Thermochemical Study of the Three Monofluorophenol Isomers
hvapt	50.30	kJ/mol	412.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	373.00 ± 3.00	K	6.10	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C372203&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Experimental and Computational Thermochemical Study of the Three Monofluorophenol Isomers: https://www.doi.org/10.1021/je9000872

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol1801.mol

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
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
hvapt:	Enthalpy of vaporization at a given temperature
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