Phenol, 2-fluoro-

Other names: 1-Fluoro-2-hydroxybenzene
2-FLUOROPHENOL
Phenol, o-fluoro-
o-Fluorophenol
Inchi: InChI=1S/C6H5FO/c7-5-3-1-2-4-6(5)8/h1-4,8H
InchiKey: HFHFGHLXUCOHLN-UHFFFAOYSA-N
Formula: C6H5FO
SMILES: Oc1ccccc1F
Mol. weight [g/mol]: 112.10
CAS: 367-12-4

Physical Properties

Property code	Value	Unit	Source
affp	788.00	kJ/mol	NIST Webbook
basg	758.00	kJ/mol	NIST Webbook
chl	-2953.00	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	52.30 ± 0.80	kJ/mol	NIST Webbook
ie	8.68 ± 0.02	eV	NIST Webbook
ie	8.97 ± 0.02	eV	NIST Webbook
ie	8.95	eV	NIST Webbook
ie	8.66 ± 0.01	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
rinpol	856.00		NIST Webbook
rinpol	128.00		NIST Webbook
rinpol	128.00		NIST Webbook
tb	424.15	K	KDB
tb	444.50 ± 0.50	K	NIST Webbook
tc	663.74	K	Joback Method
tf	289.25	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	52.30	kJ/mol	298.15	Experimental and Computational Thermochemical Study of the Three Monofluorophenol Isomers

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	444.70	K	98.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52236e+01
Coeff. B	-3.83910e+03
Coeff. C	-6.26500e+01
Temperature range (K), min.	293.00
Temperature range (K), max.	449.96

Sources

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/mol1800.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C367124&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
pvap:	Vapor 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

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