Phenol, 4-fluoro-

Other names:	4-FLUOROPHENOL
	Fluorophenol
	Phenol, p-fluoro-
	p-Fluorophenol
Inchi:	InChI=1S/C6H5FO/c7-5-1-3-6(8)4-2-5/h1-4,8H
InchiKey:	RHMPLDJJXGPMEX-UHFFFAOYSA-N
Formula:	C6H5FO
SMILES:	Oc1ccc(F)cc1
Mol. weight [g/mol]:	112.10
CAS:	371-41-5

Physical Properties

Property code	Value	Unit	Source
affp	775.00	kJ/mol	NIST Webbook
basg	747.00	kJ/mol	NIST Webbook
chs	-2914.80	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
hsub	73.90 ± 1.40	kJ/mol	NIST Webbook
hvap	43.42	kJ/mol	Joback Method
ie	8.79 ± 0.02	eV	NIST Webbook
ie	8.77	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	955.00		NIST Webbook
rinpol	955.00		NIST Webbook
tb	458.75	K	KDB
tb	458.00	K	NIST Webbook
tb	458.70	K	NIST Webbook
tc	663.74	K	Joback Method
tf	319.00 ± 4.00	K	NIST Webbook
tf	321.15	K	NIST Webbook

tf	320.40	K	Crystalline and liquid vapour pressures of the four p-monohalophenols: A thermodynamic study of their phase transitions
tf	321.35	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
cps	144.60	J/mol×K	298.15	NIST Webbook
hvapt	73.90	kJ/mol	298.15	Experimental and Computational Thermochemical Study of the Three Monofluorophenol Isomers
hvapt	48.80	kJ/mol	410.00	NIST Webbook

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/mol1799.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C371415&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Crystalline and liquid vapour pressures of the four p-monohalophenols: A thermodynamic study of their phase transitions:	https://www.doi.org/10.1016/j.jct.2013.05.047

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/56-087-4/Phenol-4-fluoro.pdf

Generated by Cheméo on 2024-10-12 03:22:43.104049651 +0000 UTC m=+3284225.741018915.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.