

Phenol, pentafluoro-

Other names:	2,3,4,5,6-PENTAFLUOROPHENOL C6F5OH Pentafluorophenol
Inchi:	InChI=1S/C6HF5O/c7-1-2(8)4(10)6(12)5(11)3(1)9/h12H
InchiKey:	XBNGYFFABRKICK-UHFFFAOYSA-N
Formula:	C6HF5O
SMILES:	Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	184.06
CAS:	771-61-9

Physical Properties

Property code	Value	Unit	Source
af	0.5020		KDB
chs	-2374.70 ± 2.00	kJ/mol	NIST Webbook
gf	-1055.14	kJ/mol	Joback Method
hf	-957.10 ± 2.00	kJ/mol	NIST Webbook
hfs	-1024.50 ± 2.00	kJ/mol	NIST Webbook
hfus	24.96	kJ/mol	Joback Method
hsub	67.40 ± 1.60	kJ/mol	NIST Webbook
hvap	52.20 ± 0.40	kJ/mol	NIST Webbook
ie	9.20 ± 0.02	eV	NIST Webbook
ie	9.37 ± 0.02	eV	NIST Webbook
log10ws	-2.68		Crippen Method
logp	2.088		Crippen Method
mcvol	86.360	ml/mol	McGowan Method
pc	4000.00	kPa	KDB
pc	3800.00 ± 300.00	kPa	NIST Webbook
rhoc	528.26 ± 5.28	kg/m ³	NIST Webbook
rhoc	533.78 ± 25.77	kg/m ³	NIST Webbook
ss	242.84	J/mol×K	NIST Webbook
ss	227.10	J/mol×K	NIST Webbook
tb	416.00	K	NIST Webbook
tb	416.00	K	NIST Webbook
tb	418.79	K	KDB
tb	416.20	K	NIST Webbook
tc	609.00 ± 6.08	K	NIST Webbook
tc	605.00 ± 5.00	K	NIST Webbook

tc	609.00	K	KDB
tf	305.90	K	KDB
tt	310.62 ± 0.02	K	NIST Webbook
tt	305.18 ± 0.02	K	NIST Webbook
vc	0.348	m ³ /kmol	KDB
zc	0.2749070		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.84	J/mol×K	642.64	Joback Method
cpg	187.58	J/mol×K	460.25	Joback Method
cpg	212.67	J/mol×K	612.24	Joback Method
cpg	208.24	J/mol×K	581.84	Joback Method
cpg	203.55	J/mol×K	551.44	Joback Method
cpg	198.55	J/mol×K	521.05	Joback Method
cpg	193.24	J/mol×K	490.65	Joback Method
cps	201.30	J/mol×K	298.15	NIST Webbook
cps	260.66	J/mol×K	298.15	NIST Webbook
hfust	16.41	kJ/mol	310.60	NIST Webbook
hfust	12.85	kJ/mol	305.18	NIST Webbook
hfust	16.41	kJ/mol	310.60	NIST Webbook
hfust	1.16	kJ/mol	287.00	NIST Webbook
hsubt	67.40 ± 1.70	kJ/mol	286.00	NIST Webbook
hvapt	44.20	kJ/mol	403.00	NIST Webbook
sfust	42.09	J/mol×K	305.18	NIST Webbook
sfust	52.83	J/mol×K	310.60	NIST Webbook
sfust	4.04	J/mol×K	287.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44320e+01
Coeff. B	-3.26908e+03
Coeff. C	-8.56360e+01
Temperature range (K), min.	312.15

Temperature range (K), max.	444.07
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Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.24983e+02
Coeff. B	-1.04583e+04
Coeff. C	-1.60813e+01
Coeff. D	9.67763e-06
Temperature range (K), min.	378.15
Temperature range (K), max.	604.40

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C771619&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1791
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/files/research/kdb/mol/mol1791.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
rhoc:	Critical density
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

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