Phenol, 2-ethyl-

Other names:	1-ETHYL-2-HYDROXYBENZENE
	1-Hydroxy-2-ethylbenzene
	2-ETHYLPHENOL
	Ethylphenol
	Florol
	NSC 10112
	PHLOROL
	Phenol, o-ethyl-
	o-Ethylphenol
	o-Hydroxyethylbenzene
Inchi:	InChI=1S/C8H10O/c1-2-7-5-3-4-6-8(7)9/h3-6,9H,2H2,1H3
InchiKey:	IXQGCWUGDFDQMF-UHFFFAOYSA-N
Formula:	C8H10O
SMILES:	CCc1ccccc1O
Mol. weight [g/mol]:	122.16
CAS:	90-00-6

Physical Properties

Property code	Value	Unit	Source
chl	-4368.39	kJ/mol	NIST Webbook
gf	-25.73	kJ/mol	Joback Method
hf	-145.20	kJ/mol	NIST Webbook
hf	-145.80	kJ/mol	KDB
hfl	-208.80	kJ/mol	NIST Webbook
hfus	16.30	kJ/mol	Joback Method
hvap	63.60	kJ/mol	NIST Webbook
hvap	64.50	kJ/mol	NIST Webbook
hvap	63.60	kJ/mol	NIST Webbook
log10ws	-1.36		Aqueous Solubility Prediction Method
logp	1.955		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method
rinpol	1115.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1175.00		NIST Webbook

rinpol	1148.00	NIST Webbook
rinpol	1113.00	NIST Webbook
rinpol	1113.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1114.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1160.00	NIST Webbook
rinpol	1137.90	NIST Webbook
rinpol	1136.50	NIST Webbook
rinpol	1136.20	NIST Webbook
rinpol	1148.70	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1177.00	NIST Webbook
rinpol	190.00	NIST Webbook
rinpol	189.73	NIST Webbook
rinpol	188.30	NIST Webbook
rinpol	1138.00	NIST Webbook
rinpol	1108.00	NIST Webbook
rinpol	1112.80	NIST Webbook
rinpol	1104.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1118.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	190.21	NIST Webbook
rinpol	1112.00	NIST Webbook
rinpol	1112.00	NIST Webbook
rinpol	1113.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1106.00	NIST Webbook
rinpol	1148.70	NIST Webbook
ripol	2079.00	NIST Webbook
ripol	2068.00	NIST Webbook
ripol	2054.00	NIST Webbook
ripol	2059.00	NIST Webbook
ripol	2050.00	NIST Webbook
ripol	2071.00	NIST Webbook
ripol	2028.00	NIST Webbook
ripol	2084.00	NIST Webbook
ripol	2063.00	NIST Webbook
ripol	2068.00	NIST Webbook

ripol	2044.00		NIST Webbook
ripol	2044.00		NIST Webbook
ripol	2079.00		NIST Webbook
ripol	2063.00		NIST Webbook
ripol	2069.00		NIST Webbook
tb	469.20	K	NIST Webbook
tb	480.20	K	NIST Webbook
tb	480.65 ± 3.00	K	NIST Webbook
tb	480.15 ± 3.00	K	NIST Webbook
tb	480.15 ± 2.00	K	NIST Webbook
tb	474.65 ± 3.00	K	NIST Webbook
tb	478.05 ± 2.00	K	NIST Webbook
tb	479.15 ± 4.00	K	NIST Webbook
tb	481.15 ± 3.00	K	NIST Webbook
tb	474.65 ± 4.00	K	NIST Webbook
tb	477.65 ± 3.00	K	NIST Webbook
tb	480.65 ± 3.00	K	NIST Webbook
tb	478.05 ± 3.00	K	NIST Webbook
tb	477.67	K	KDB
tb	482.65 ± 3.00	K	NIST Webbook
tc	702.95 ± 0.30	K	NIST Webbook
tc	703.00	K	KDB
tf	414.65	K	NIST Webbook
tf	255.15 ± 5.00	K	NIST Webbook
tf	255.15 ± 10.00	K	NIST Webbook
tf	269.84 ± 0.10	K	NIST Webbook
tf	261.65	K	Aqueous Solubility Prediction Method
tf	291.00	K	KDB
tf	250.15 ± 10.00	K	NIST Webbook
tf	250.15 ± 10.00	K	NIST Webbook
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.56	J/mol×K	715.75	Joback Method
cpg	224.79	J/mol×K	489.74	Joback Method
cpg	236.73	J/mol×K	527.41	Joback Method
cpg	247.77	J/mol×K	565.08	Joback Method
cpg	258.00	J/mol×K	602.74	Joback Method

cpg	267.49	J/mol×K	640.41	Joback Method
cpg	276.31	J/mol×K	678.08	Joback Method
dvisc	0.0000969	Pa×s	489.74	Joback Method
dvisc	0.0051808	Pa×s	318.06	Joback Method
dvisc	0.0020303	Pa×s	346.67	Joback Method
dvisc	0.0009178	Pa×s	375.29	Joback Method
dvisc	0.0004643	Pa×s	403.90	Joback Method
dvisc	0.0002571	Pa×s	432.51	Joback Method
dvisc	0.0001531	Pa×s	461.13	Joback Method
hsubt	80.30 ± 0.50	kJ/mol	297.50	NIST Webbook
hvapt	43.10	kJ/mol	406.50	NIST Webbook
hvapt	50.50	kJ/mol	457.00	NIST Webbook
hvapt	63.50	kJ/mol	297.50	NIST Webbook
hvapt	51.60	kJ/mol	419.50	NIST Webbook
hvapt	51.40	kJ/mol	406.50	NIST Webbook
hvapt	49.50	kJ/mol	406.50	NIST Webbook
hvapt	48.60	kJ/mol	406.50	NIST Webbook
hvapt	47.00	kJ/mol	406.50	NIST Webbook
rhol	1037.00	kg/m3	273.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53904e+01
Coeff. B	-4.35252e+03
Coeff. C	-7.39420e+01
Temperature range (K), min.	362.14
Temperature range (K), max.	505.79

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	-2.29537e+02
Coeff. B	3.61538e+03
Coeff. C	3.82332e+01
Coeff. D	-4.08192e-05
Temperature range (K), min.	350.00
Temperature range (K), max.	500.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=871
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Liquid-Liquid Equilibrium Measurements for Model Systems Related to Catalytic Fast Pyrolysis of Biomass:	https://www.doi.org/10.1021/acs.jced.6b00625
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90006&Units=SI
Effect of Isomers on Partition Coefficients for Phenolic Compounds in the 1-Butyl-3-methylimidazolium Hexafluorophosphate + Water Two-Phase System:	https://www.doi.org/10.1021/je100016z
KDB:	https://www.cheric.org/files/research/kdb/mol/mol871.mol

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume