Phenol, 3-ethyl-

Other names:	1-ETHYL-3-HYDROXYBENZENE
	1-Hydroxy-3-ethylbenzene
	3-ETHYLPHENOL
	Phenol, m-ethyl-
	m-Ethylphenol
Inchi:	InChI=1S/C8H10O/c1-2-7-4-3-5-8(9)6-7/h3-6,9H,2H2,1H3
InchiKey:	HMNKTRSOROOSPP-UHFFFAOYSA-N
Formula:	C8H10O
SMILES:	CCc1cccc(O)c1
Mol. weight [g/mol]:	122.16
CAS:	620-17-7

Physical Properties

Property code	Value	Unit	Source
chl	-4362.90 ± 1.50	kJ/mol	NIST Webbook
gf	-25.73	kJ/mol	Joback Method
hf	-146.60	kJ/mol	KDB
hf	-146.20 ± 1.70	kJ/mol	NIST Webbook
hfl	-214.30 ± 1.60	kJ/mol	NIST Webbook
hfus	16.30	kJ/mol	Joback Method
hvap	68.20 ± 0.10	kJ/mol	NIST Webbook
hvap	68.10	kJ/mol	NIST Webbook
log10ws	-1.82		Crippen Method
logp	1.955		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method
rinpol	1143.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1142.70		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1183.70		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1167.00		NIST Webbook

rinpol	1169.00	NIST Webbook
rinpol	1138.00	NIST Webbook
rinpol	1195.00	NIST Webbook
rinpol	1175.00	NIST Webbook
rinpol	1176.00	NIST Webbook
rinpol	1135.00	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	1130.00	NIST Webbook
rinpol	1172.00	NIST Webbook
rinpol	1139.00	NIST Webbook
rinpol	1138.00	NIST Webbook
rinpol	1170.00	NIST Webbook
rinpol	1169.00	NIST Webbook
rinpol	1146.00	NIST Webbook
rinpol	1176.00	NIST Webbook
rinpol	1170.00	NIST Webbook
rinpol	1147.00	NIST Webbook
rinpol	1160.00	NIST Webbook
rinpol	197.80	NIST Webbook
rinpol	190.60	NIST Webbook
rinpol	194.60	NIST Webbook
rinpol	196.96	NIST Webbook
rinpol	196.80	NIST Webbook
rinpol	196.96	NIST Webbook
rinpol	196.80	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1160.00	NIST Webbook
rinpol	1183.70	NIST Webbook
rinpol	1167.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1189.00	NIST Webbook
rinpol	1189.00	NIST Webbook
ripol	2191.00	NIST Webbook
ripol	2190.00	NIST Webbook
ripol	2195.00	NIST Webbook
ripol	2218.00	NIST Webbook
ripol	2151.00	NIST Webbook
ripol	2141.00	NIST Webbook
ripol	2150.00	NIST Webbook
ripol	2195.00	NIST Webbook
ripol	2189.00	NIST Webbook

ripol	2188.00		NIST Webbook
ripol	2189.00		NIST Webbook
ripol	2190.00		NIST Webbook
ripol	2205.00		NIST Webbook
ripol	2168.00		NIST Webbook
ripol	2169.00		NIST Webbook
ripol	2171.00		NIST Webbook
ripol	2210.00		NIST Webbook
ripol	2170.00		NIST Webbook
ripol	2167.00		NIST Webbook
ripol	2171.00		NIST Webbook
ripol	2194.00		NIST Webbook
ripol	2194.00		NIST Webbook
ripol	2181.00		NIST Webbook
ripol	2170.00		NIST Webbook
tb	491.57	K	KDB
tc	718.80	K	KDB
tc	716.45 ± 0.15	K	NIST Webbook
tf	269.15 ± 2.00	K	NIST Webbook
tf	269.00	K	KDB
tf	269.15 ± 2.00	K	NIST Webbook
tf	269.15 ± 2.00	K	NIST Webbook
tf	269.15 ± 2.00	K	NIST Webbook
tf	269.15 ± 2.00	K	NIST Webbook
tf	268.65 ± 1.00	K	NIST Webbook
tf	269.15 ± 2.00	K	NIST Webbook
tf	269.15 ± 2.00	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
hvapt	48.80	kJ/mol	417.50	NIST Webbook
hvapt	53.10	kJ/mol	474.00	NIST Webbook
hvapt	68.10	kJ/mol	300.00	NIST Webbook
hvapt	58.30	kJ/mol	417.50	NIST Webbook
hvapt	56.50	kJ/mol	417.50	NIST Webbook
hvapt	55.20	kJ/mol	417.50	NIST Webbook
hvapt	53.70	kJ/mol	417.50	NIST Webbook
rhol	1025.00	kg/m3	273.00	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	382.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56730e+01
Coeff. B	-4.54561e+03
Coeff. C	-7.78060e+01
Temperature range (K), min.	373.26
Temperature range (K), max.	516.51

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.13752e+02
Coeff. B	-1.18918e+04
Coeff. C	-1.38880e+01
Coeff. D	4.72667e-06

Temperature range (K), min.	370.00
Temperature range (K), max.	502.15

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol872.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=872
Effect of Isomers on Partition Coefficients for Phenolic Compounds	https://www.doi.org/10.1021/je100016z
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C620177&Units=SI
In the 1-Butyl-3-methylimidazolium Hexafluorophosphate + Water Two-Phase System:	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Liquid-Liquid Equilibrium Measurements for Model Systems	https://www.doi.org/10.1021/acs.jced.6b00625
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Related to Catalytic Fast Pyrolysis of Biomass:	
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume