

Phenol, 4-ethyl-

Other names:	1-ETHYL-4-HYDROXYBENZENE 1-Hydroxy-4-ethylbenzene 4-ETHYLPHENOL 4-hydroxyphenylethane Paraethylphenol Phenol, p-ethyl- p-Ethylphenol
Inchi:	InChI=1S/C8H10O/c1-2-7-3-5-8(9)6-4-7/h3-6,9H,2H2,1H3
InchiKey:	HXDOZKJGKXYMEW-UHFFFAOYSA-N
Formula:	C8H10O
SMILES:	CCc1ccc(O)cc1
Mol. weight [g/mol]:	122.16
CAS:	123-07-9

Physical Properties

Property code	Value	Unit	Source
chs	-4352.82 ± 0.92	kJ/mol	NIST Webbook
gf	-25.73	kJ/mol	Joback Method
hf	-144.30 ± 1.10	kJ/mol	NIST Webbook
hf	-144.70	kJ/mol	KDB
hfs	-224.40 ± 1.00	kJ/mol	NIST Webbook
hfus	16.30	kJ/mol	Joback Method
hsub	80.10	kJ/mol	NIST Webbook
hsub	80.30 ± 0.10	kJ/mol	NIST Webbook
hvap	48.69	kJ/mol	Joback Method
ie	7.84	eV	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	1145.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1161.00		NIST Webbook

rinpol	1170.00	NIST Webbook
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rinpol	1141.00	NIST Webbook
rinpol	1181.00	NIST Webbook
rinpol	1192.00	NIST Webbook
rinpol	1178.00	NIST Webbook
rinpol	1137.00	NIST Webbook
rinpol	1171.00	NIST Webbook
rinpol	1133.00	NIST Webbook
rinpol	1141.00	NIST Webbook
rinpol	1169.00	NIST Webbook
rinpol	1170.00	NIST Webbook
rinpol	1188.00	NIST Webbook
rinpol	1137.00	NIST Webbook
rinpol	1142.00	NIST Webbook
rinpol	1141.00	NIST Webbook
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rinpol	1130.00	NIST Webbook
rinpol	1165.80	NIST Webbook
ripol	2198.00	NIST Webbook
ripol	2180.00	NIST Webbook
ripol	2143.00	NIST Webbook
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ripol	2172.00	NIST Webbook
ripol	2207.00	NIST Webbook
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ripol	2186.00	NIST Webbook
ripol	2205.00	NIST Webbook
ripol	2209.00	NIST Webbook
ripol	2195.00	NIST Webbook
ripol	2214.00	NIST Webbook
ripol	2209.00	NIST Webbook
ripol	2207.00	NIST Webbook
ripol	2208.00	NIST Webbook
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ripol	2195.00	NIST Webbook
ripol	2142.00	NIST Webbook
ripol	2193.00	NIST Webbook
ripol	2175.00	NIST Webbook
ripol	2160.00	NIST Webbook
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ripol	2204.00	NIST Webbook
ripol	2185.00	NIST Webbook
ripol	2198.00	NIST Webbook
ripol	2190.00	NIST Webbook
ripol	2152.00	NIST Webbook
ripol	2153.00	NIST Webbook
ripol	2157.00	NIST Webbook
ripol	2188.00	NIST Webbook

tb	484.15 ± 3.00	K	NIST Webbook
tb	487.65 ± 4.00	K	NIST Webbook
tb	486.65 ± 3.00	K	NIST Webbook
tb	488.65 ± 3.00	K	NIST Webbook
tb	490.40 ± 2.00	K	NIST Webbook
tb	491.15 ± 3.00	K	NIST Webbook
tb	490.15 ± 3.00	K	NIST Webbook
tb	492.00 ± 0.60	K	NIST Webbook
tb	486.65 ± 4.00	K	NIST Webbook
tb	492.45 ± 3.00	K	NIST Webbook
tb	492.15 ± 3.00	K	NIST Webbook
tb	491.35 ± 2.00	K	NIST Webbook
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tb	492.15 ± 2.00	K	NIST Webbook
tb	492.15 ± 2.00	K	NIST Webbook
tb	492.15 ± 2.00	K	NIST Webbook
tb	492.20	K	NIST Webbook
tb	491.13	K	KDB
tc	716.40	K	KDB
tc	716.45 ± 0.80	K	NIST Webbook
tf	319.15 ± 2.00	K	NIST Webbook
tf	318.23	K	KDB
tf	318.21 ± 0.05	K	NIST Webbook
tf	317.95 ± 2.00	K	NIST Webbook
tf	317.65 ± 2.00	K	NIST Webbook
tf	318.15 ± 2.00	K	NIST Webbook
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tf	318.65 ± 2.00	K	NIST Webbook
tf	318.15 ± 2.00	K	NIST Webbook
tf	318.65 ± 2.00	K	NIST Webbook
tf	318.65 ± 2.00	K	NIST Webbook
tf	318.65 ± 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	276.31	J/mol×K	678.08	Joback Method
cpg	267.49	J/mol×K	640.41	Joback Method
cpg	258.00	J/mol×K	602.74	Joback Method
cpg	247.77	J/mol×K	565.08	Joback Method
cpg	236.73	J/mol×K	527.41	Joback Method
cpg	224.79	J/mol×K	489.74	Joback Method
cps	206.90	J/mol×K	298.15	NIST Webbook
dvisc	0.0002571	Pa×s	432.51	Joback Method
dvisc	0.0051808	Pa×s	318.06	Joback Method
dvisc	0.0000969	Pa×s	489.74	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	0.0001531	Pa×s	461.13	Joback Method
hvapt	53.20	kJ/mol	473.50	NIST Webbook
hvapt	47.60	kJ/mol	420.00	NIST Webbook
hvapt	51.30	kJ/mol	420.00	NIST Webbook
hvapt	53.80	kJ/mol	420.00	NIST Webbook
hvapt	56.50	kJ/mol	420.00	NIST Webbook
hvapt	54.70	kJ/mol	420.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.55378e+01
Coeff. B	-4.50225e+03
Coeff. C	-7.76870e+01
Temperature range (K), min.	372.91
Temperature range (K), max.	517.95

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	9.91252e+00
Coeff. B	-6.88694e+03
Coeff. C	1.59162e+00
Coeff. D	-4.83517e-06
Temperature range (K), min.	318.23

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123079&Units=SI
Effect of Isomers on Partition Coefficients for Phenolic Compounds	https://www.doi.org/10.1021/je100016z
Joback Method	https://en.wikipedia.org/wiki/Joback_method
1-methyl-2-methylimidazolium Hexafluorophosphate + Water	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method	https://www.doi.org/10.1021/acs.jced.6b00625
Liquid-Liquid Equilibrium Measurements for Model Systems	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
The Yaws Handbook of Vapor Pressure	https://www.cheric.org/files/research/kdb/mol/mol873.mol
Related to Catalytic Fast Pyrolysis of Biomass:	
KDB:	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=873

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
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
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
pvap:	Vapor pressure
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

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