

Phenol

Other names:

Acide carbolique
Baker's P & S liquid & Ointment
Baker's P and S Liquid and Ointment
Benzene, hydroxy-
Benzenol
Carbolic acid
Carbolsaure
Fenol
Fenolo
Hydroxybenzene
Izal
Monohydroxybenzene
Monophenol
NA 2821
NCI-C50124
NSC 36808
Oxybenzene
Paoscle
PhOH
Phenic acid
Phenic alcohol
Phenol alcohol
Phenol, molten
Phenole
Phenyl alcohol
Phenyl hydrate
Phenyl hydroxide
Phenylic acid
Phenylic alcohol
Rcra waste number U188
UN 1671
UN 2312
UN 2821

Inchi: InChI=1S/C6H6O/c7-6-4-2-1-3-5-6/h1-5,7H

InchiKey: ISWSIDIOOBQZ-UHFFFAOYSA-N

Formula: C6H6O

SMILES: Oc1ccccc1

Mol. weight [g/mol]: 94.11

CAS: 108-95-2

Physical Properties

Property code	Value	Unit	Source
af	0.4380		KDB
affp	817.30	kJ/mol	NIST Webbook
aigt	988.15	K	KDB
basg	786.30	kJ/mol	NIST Webbook
chs	-3054.70	kJ/mol	NIST Webbook
chs	-3053.60 ± 0.30	kJ/mol	NIST Webbook
chs	-3053.50 ± 0.67	kJ/mol	NIST Webbook
chs	-3055.80	kJ/mol	NIST Webbook
chs	-3067.00	kJ/mol	NIST Webbook
chs	-3066.04	kJ/mol	NIST Webbook
dm	1.60	debye	KDB
fll	1.70	% in Air	KDB
flu	8.60	% in Air	KDB
fpc	358.15	K	KDB
fpo	352.59	K	KDB
gf	-32.90	kJ/mol	KDB
gyrad	3.5500		KDB
hf	-94.20	kJ/mol	NIST Webbook
hf	-96.36 ± 0.59	kJ/mol	NIST Webbook
hf	-96.42	kJ/mol	KDB
hf	-95.30	kJ/mol	NIST Webbook
hf	-96.44 ± 0.63	kJ/mol	NIST Webbook
hfs	-162.80 ± 1.00	kJ/mol	NIST Webbook
hfs	-165.10 ± 1.30	kJ/mol	NIST Webbook
hfs	-165.00	kJ/mol	NIST Webbook
hfs	-163.90	kJ/mol	NIST Webbook
hfus	11.51	kJ/mol	Joback Method
hsub	68.60	kJ/mol	NIST Webbook
hsub	68.66 ± 0.50	kJ/mol	NIST Webbook
hsub	68.70	kJ/mol	NIST Webbook
hsub	69.70 ± 0.90	kJ/mol	NIST Webbook
hvap	58.80	kJ/mol	NIST Webbook
ie	8.56	eV	NIST Webbook
ie	8.55	eV	NIST Webbook
ie	8.47 ± 0.02	eV	NIST Webbook
ie	8.21	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
ie	8.49	eV	NIST Webbook
ie	8.51 ± 0.00	eV	NIST Webbook

ie	8.51 ± 0.00	eV	NIST Webbook
ie	9.10 ± 0.10	eV	NIST Webbook
ie	8.37	eV	NIST Webbook
ie	8.67	eV	NIST Webbook
ie	8.73	eV	NIST Webbook
ie	8.69	eV	NIST Webbook
ie	8.56	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
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ie	8.52 ± 0.02	eV	NIST Webbook
ie	8.50 ± 0.01	eV	NIST Webbook
ie	8.52	eV	NIST Webbook
ie	8.48 ± 0.05	eV	NIST Webbook
ie	8.69	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.49 ± 0.02	eV	NIST Webbook
log10ws	0.00		Aqueous Solubility Prediction Method
log10ws	0.00		Estimated Solubility Method
logp	1.392		Crippen Method
mcvol	77.510	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=3)		KDB
pc	5930.00 ± 78.45	kPa	NIST Webbook
pc	6130.16 ± 81.06	kPa	NIST Webbook
pc	5670.00	kPa	Vapor-Liquid Critical Properties of Phenol and (C8 to C10) Phenylalkanols
pc	6130.00	kPa	KDB
rinpol	950.00		NIST Webbook
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ss	144.01	J/mol×K	NIST Webbook
ss	142.70	J/mol×K	NIST Webbook
tb	455.35 ± 0.30	K	NIST Webbook
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tb	458.00 ± 0.30	K	NIST Webbook

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tc	694.30 ± 0.40	K	NIST Webbook
tc	694.25 ± 0.15	K	NIST Webbook
tc	694.20	K	KDB
tf	314.05	K	Solid-liquid equilibria and the physical properties of binary systems of diphenyl carbonate, dimethyl carbonate, methyl phenyl carbonate, anisole, methanol and phenol
tf	314.00	K	KDB
tf	314.30	K	Aqueous Solubility Prediction Method
tf	314.85	K	(Solid + liquid) phase equilibria and solid-compound formation in (N-methyl-2-pyrrolidinone + phenol, or 3,5-dimethylphenol)

tf	314.10	K	The solid-liquid equililibrium, excess molar volume and refractive deviation properties of binary systems containing dimethyl carbonate, anisole and phenol
tf	314.15	K	Liquid pharmaceuticals formulation by eutectic formation
tt	314.06 ± 0.01	K	NIST Webbook
vc	0.229	m3/kmol	KDB
zc	0.2432060		KDB
zra	0.28		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.52	J/mol×K	439.00	Joback Method
cpg	155.59	J/mol×K	477.67	Joback Method
cpg	164.73	J/mol×K	516.34	Joback Method
cpg	173.03	J/mol×K	555.01	Joback Method
cpg	180.59	J/mol×K	593.67	Joback Method
cpg	187.47	J/mol×K	632.34	Joback Method
cpg	193.78	J/mol×K	671.01	Joback Method
cps	133.09	J/mol×K	295.80	NIST Webbook
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dvisc	0.0002857	Pa×s	413.00	Joback Method
dvisc	0.0005026	Pa×s	387.00	Joback Method
dvisc	0.0020238	Pa×s	335.00	Joback Method
dvisc	0.0135969	Pa×s	283.00	Joback Method
dvisc	0.0048418	Pa×s	309.00	Joback Method
hfust	12.12	kJ/mol	314.13	NIST Webbook
hfust	11.51	kJ/mol	314.00	NIST Webbook
hfust	11.51	kJ/mol	314.06	NIST Webbook
hfust	10.58	kJ/mol	312.70	NIST Webbook
hfust	11.51	kJ/mol	314.00	NIST Webbook
hsubt	68.70 ± 0.50	kJ/mol	297.50	NIST Webbook

hsubt	68.20	kJ/mol	293.00	NIST Webbook
hsubt	68.10	kJ/mol	291.50	NIST Webbook
hsubt	65.30 ± 3.30	kJ/mol	280.50	NIST Webbook
hsubt	67.80	kJ/mol	291.50	NIST Webbook
hvapt	43.80	kJ/mol	572.50	NIST Webbook
hvapt	45.61	kJ/mol	454.90	KDB
hvapt	53.20	kJ/mol	377.00	NIST Webbook
hvapt	57.40	kJ/mol	354.50	NIST Webbook
hvapt	50.90	kJ/mol	421.50	NIST Webbook
hvapt	48.10	kJ/mol	434.00	NIST Webbook
hvapt	51.40	kJ/mol	417.50	NIST Webbook
hvapt	51.30	kJ/mol	428.00	NIST Webbook
hvapt	46.80	kJ/mol	487.50	NIST Webbook
hvapt	49.50	kJ/mol	555.00	NIST Webbook
pvap	13.15	kPa	393.15	Vapor-Liquid Equilibrium for Phenol + r-Methyl Benzyl Alcohol and 2-Ethoxyethanol + n-Butyl Formate
pvap	5.53	kPa	373.10	Vapor-Liquid Equilibria on Four Binary Systems: 2-Phenylpropionaldehyde + Phenol, Propylene Glycol Monomethyl Ether + Nitroethane, Dimethyl Ether + Propylene, and N-Butyric Acid + Propionic Acid
pvap	39.18	kPa	423.15	Vapor-Liquid Equilibria on Four Binary Systems: 2-Phenylpropionaldehyde + Phenol, Propylene Glycol Monomethyl Ether + Nitroethane, Dimethyl Ether + Propylene, and N-Butyric Acid + Propionic Acid
pvap	5.54	kPa	373.15	Vapor-Liquid Equilibrium for Phenol + r-Methyl Benzyl Alcohol and 2-Ethoxyethanol + n-Butyl Formate

pvap	2.04	kPa	353.15	Vapor-Liquid Equilibrium for Phenol + r-Methyl Benzyl Alcohol and 2-Ethoxyethanol + n-Butyl Formate
pvap	5.51	kPa	373.10	Vapor-Liquid Equilibria on Seven Binary Systems: Ethylene Oxide + 2-Methylpropane; Acetophenone + Phenol; cis-1,3-Dichloropropene + 1,2-Dichloropropane; 1,5-Hexadiene + Allyl Chloride; Isopropyl Acetate + Acetonitrile; Vinyl Chloride + Methyl Chloride; and 1,4-Butanediol + c-Butyrolactone
pvap	53.23	kPa	433.15	Vapor-Liquid Equilibria on Seven Binary Systems: Ethylene Oxide + 2-Methylpropane; Acetophenone + Phenol; cis-1,3-Dichloropropene + 1,2-Dichloropropane; 1,5-Hexadiene + Allyl Chloride; Isopropyl Acetate + Acetonitrile; Vinyl Chloride + Methyl Chloride; and 1,4-Butanediol + c-Butyrolactone
rfi	1.54050		314.15	Liquid-liquid equilibria of water + solutes (acetic acid/acetol/furfural/guaiacol/methanol/phenol/propanal) + solvents (isopropyl acetate/toluene) ternary systems for pyrolysis oil fractionation

rhoI	1054.10	kg/m3	318.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1045.50	kg/m3	328.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1058.30	kg/m3	313.15	Vapor-Liquid Equilibria in Ternary Systems of Toluene or Octane + Phenols + Water
rhoI	1036.79	kg/m3	338.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1032.40	kg/m3	343.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1058.30	kg/m3	313.15	Liquid-Liquid(-Liquid) Equilibria in Ternary Systems of Aliphatic Hydrocarbons (Heptane or Octane) + Phenols + Water
rhoI	1049.81	kg/m3	323.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model

rhoI	1058.30	kg/m3	313.15	Liquid-Liquid Equilibria in Ternary Systems of Aromatic Hydrocarbons (Toluene or Ethylbenzene) + Phenols + Water
rhoI	1058.10	kg/m3	314.50	Ternary and Quaternary Liquid-Liquid Equilibria for Systems of Methyl Butyl Ketone + Water + Hydroquinone + Phenol at 313.2 K and Atmospheric Pressure
rhoI	1058.51	kg/m3	298.15	Ternary liquid-liquid equilibria and binary excess and deviation properties at constant temperature for mixtures of dimethyl carbonate, anisole, methanol, phenol and water
rhoI	1061.00	kg/m3	314.45	Liquid liquid equilibria for the quaternary system methyl isobutyl ketone water phenol hydroquinone
rhoI	1041.16	kg/m3	333.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1058.51	kg/m3	313.15	Liquid Liquid Equilibria for Ternary Mixtures of Methylphenyl Carbonate, Dimethyl Carbonate, Diphenyl Carbonate, Anisole, Methanol, Phenol, and Water at Several Temperatures

[illegible]

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Legend

af:	Acentric Factor
affp:	Proton affinity
aignt:	Autoignition Temperature
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
fl:	Lower Flammability Limit
flu:	Upper Flammability Limit
fpc:	Flash Point (Closed Cup Method)
fpo:	Flash Point (Open Cup Method)
gf:	Standard Gibbs free energy of formation
gyrad:	Radius of Gyration
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhof:	Liquid Density
ripol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
srf:	Surface Tension
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
zra:	Rackett Parameter

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