

Phenol, 2-methoxy-

Other names:	1-Hydroxy-2-methoxybenzene
	2-Hydroxyanisole
	2-Methoxy phenol (guaiacol)
	2-Methoxyphenol
	2-methoxyphenol (guaiacol)
	Anastil
	Catechol monomethyl ether
	Guaiacol
	Guaiastil
	Guaicol
	Guaicolina
	Guajakol
	Guajol
	Guasol
	Methylcatachol
	Methylcatechol
	NSC 3815
	O-Methyl catechol
	Phenol, o-methoxy-
	Pyrocatechol monomethyl ether
	Pyroguaiac acid
	guaiacol (2-methoxyphenol)
	guiacol
	o-Guaiacol
	o-Guiacol
	o-Hydroxyanisole
	o-Methoxyphenol
	ortho-Guaiacol
Inchi:	InChI=1S/C7H8O2/c1-9-7-5-3-2-4-6(7)8/h2-5,8H,1H3
InchiKey:	LHGVFZTZFXWLCP-UHFFFAOYSA-N
Formula:	C7H8O2
SMILES:	COc1ccccc1O
Mol. weight [g/mol]:	124.14
CAS:	90-05-1

Physical Properties

Property code	Value	Unit	Source
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gf	-139.15	kJ/mol	Joback Method
hf	-260.81	kJ/mol	Joback Method
hfus	14.90	kJ/mol	Joback Method
hvap	62.60 ± 0.50	kJ/mol	NIST Webbook
log10ws	-1.96		Estimated Solubility Method
log10ws	-1.96		Aqueous Solubility Prediction Method
logp	1.401		Crippen Method
mcvol	97.470	ml/mol	McGowan Method
pc	4910.80	kPa	Joback Method
rinpol	1071.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	180.07		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1090.00		NIST Webbook
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ripol	1884.00		NIST Webbook
tb	478.30 ± 0.50	K	NIST Webbook
tb	478.20 ± 0.50	K	NIST Webbook
tb	478.20 ± 0.60	K	NIST Webbook
tb	478.20	K	NIST Webbook
tb	478.25	K	Isobaric (vapour + liquid) equilibria of binary systems containing butyl acetate for the separation of methoxy aromatic compounds (anisole and guaiacol) from biomass fast pyrolysis oil
tb	478.10	K	Isobaric vapour + liquid equilibria for three binary systems (toluene + anisole, nbutylbenzene + anisole, and guaiacol + anisole) at 101.33 kPa
tb	478.15 ± 1.00	K	NIST Webbook
tc	716.68	K	Joback Method
tf	301.15 ± 0.40	K	NIST Webbook
tf	301.25 ± 0.40	K	NIST Webbook
tf	301.45 ± 0.60	K	NIST Webbook
tf	302.65	K	Aqueous Solubility Prediction Method
vc	0.303	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.19	J/mol×K	716.68	Joback Method
cpg	215.86	J/mol×K	527.18	Joback Method
cpg	225.57	J/mol×K	565.08	Joback Method
cpg	234.59	J/mol×K	602.98	Joback Method
cpg	243.00	J/mol×K	640.88	Joback Method
cpg	250.84	J/mol×K	678.78	Joback Method
cpg	205.43	J/mol×K	489.28	Joback Method
dvisc	0.0001338	Pa×s	462.57	Joback Method
dvisc	0.0002167	Pa×s	435.86	Joback Method
dvisc	0.0003736	Pa×s	409.15	Joback Method
dvisc	0.0006951	Pa×s	382.44	Joback Method

dvisc	0.0014199	Pa×s	355.73	Joback Method
dvisc	0.0000871	Pa×s	489.28	Joback Method
dvisc	0.0032569	Pa×s	329.02	Joback Method
hvapt	52.70	kJ/mol	428.50	NIST Webbook
hvapt	52.70	kJ/mol	416.50	NIST Webbook
pvap	40.30	kPa	443.15	Isothermal Vapor-Liquid Equilibria for Binary Mixtures Composed of the Closely Boiling Compounds 1,2-Dimethoxybenzene and 2-Methoxyphenol with an Adducted Agent: tert-Butanol or Morpholine
pvap	7.08	kPa	393.15	Isothermal Vapor-Liquid Equilibria for Binary Mixtures Composed of the Closely Boiling Compounds 1,2-Dimethoxybenzene and 2-Methoxyphenol with an Adducted Agent: tert-Butanol or Morpholine
pvap	25.30	kPa	428.15	Isothermal Vapor-Liquid Equilibria for Binary Mixtures Composed of the Closely Boiling Compounds 1,2-Dimethoxybenzene and 2-Methoxyphenol with an Adducted Agent: tert-Butanol or Morpholine
pvap	2.98	kPa	373.15	Isothermal Vapor-Liquid Equilibria for Binary Mixtures Composed of the Closely Boiling Compounds 1,2-Dimethoxybenzene and 2-Methoxyphenol with an Adducted Agent: tert-Butanol or Morpholine

pvap	4.69	kPa	383.15	Isothermal Vapor-Liquid Equilibria for Binary Mixtures Composed of the Closely Boiling Compounds 1,2-Dimethoxybenzene and 2-Methoxyphenol with an Adducted Agent: tert-Butanol or Morpholine
pvap	15.20	kPa	413.15	Isothermal Vapor-Liquid Equilibria for Binary Mixtures Composed of the Closely Boiling Compounds 1,2-Dimethoxybenzene and 2-Methoxyphenol with an Adducted Agent: tert-Butanol or Morpholine
rfi	1.54410		293.15	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	1099.74	kg/m3	328.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1104.63	kg/m3	323.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model

rhoI	1094.84	kg/m3	333.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1089.94	kg/m3	338.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1085.02	kg/m3	343.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1109.51	kg/m3	318.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
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rhoI	1124.11	kg/m3	303.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model

rhoI	1128.96	kg/m3	298.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1138.64	kg/m3	288.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhoI	1133.81	kg/m3	293.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.61703e+01
Coeff. B	-5.07444e+03
Coeff. C	-3.89280e+01
Temperature range (K), min.	358.42
Temperature range (K), max.	506.24

Sources

Solubilities and Thermodynamic Properties of Carbon Dioxide in Phase equilibria of phenolic compounds in water or ethanol: Aqueous Solubility Prediction Method: <https://www.doi.org/10.1021/acs.jced.6b01013>

Phase equilibria of phenolic compounds in water or ethanol: Aqueous Solubility Prediction Method: <https://www.doi.org/10.1016/j.fluid.2017.09.008>

Phase equilibria of phenolic compounds in water or ethanol: Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C90051&Units=SI>

Extraction of phenolic compounds from aqueous solution using choline bis(trifluoromethylsulfonyl)imide: <https://www.doi.org/10.1016/j.fluid.2017.04.022>

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