Benzene, 1,2-dimethoxy-

Other names:	1,2-Dimethoxybenzene
	1,2-Dimethoxybenzene (Veratrol)
	1,2-Dimethoxybenzene (veratroI)
	1,2-Dimethoxybenzene (veratrole)
	2-Methoxyanisole
	Benzene, o-dimethoxy-
	Catechol dimethyl ether
	Dimethylether pyrokatechinu
	Methylguaiacol
	NSC 16934
	O,O-Dimethyl catechol
	Orthodimethoxybenzene
	Pyrocatechol dimethyl ether
	Veratrol
	Veratrole
	o-Dimethoxybenzene
Inchi:	InChI=1S/C8H10O2/c1-9-7-5-3-4-6-8(7)10-2/h3-6H,1-2H3
InchiKey:	ABDKAPXRBAPSQN-UHFFFAOYSA-N
Formula:	C8H10O2
SMILES:	COc1ccccc1OC
Mol. weight [g/mol]:	138.16
CAS:	91-16-7

Physical Properties

Property code	Value	Unit	Source
chl	-4286.90 ± 2.10	kJ/mol	NIST Webbook
gf	-90.74	kJ/mol	Joback Method
hf	-247.83	kJ/mol	Joback Method
hfus	12.50	kJ/mol	Joback Method
hvap	68.10 ± 1.40	kJ/mol	NIST Webbook
hvap	66.90	kJ/mol	NIST Webbook
ie	8.17	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
ie	7.80 ± 0.15	eV	NIST Webbook

log10ws	-1.31		Aqueous Solubility Prediction Method
logp	1.704		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
rinpol	1110.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1153.80		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	200.73		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1111.20		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1117.00		NIST Webbook

rinpol	1147.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1111.20		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1131.00		NIST Webbook
ripol	1715.00		NIST Webbook
ripol	1703.00		NIST Webbook
ripol	1706.00		NIST Webbook
ripol	1727.00		NIST Webbook
ripol	1699.00		NIST Webbook
ripol	1703.00		NIST Webbook
ripol	1718.00		NIST Webbook
ripol	1752.00		NIST Webbook
ripol	1753.00		NIST Webbook
ripol	1699.00		NIST Webbook
ripol	1715.00		NIST Webbook
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ripol	1731.00		NIST Webbook
ripol	1704.00		NIST Webbook
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ripol	1721.00		NIST Webbook
ripol	1727.00		NIST Webbook
ripol	1716.00		NIST Webbook
ripol	1732.00		NIST Webbook
ripol	1699.00		NIST Webbook
ripol	1720.00		NIST Webbook
ripol	1737.00		NIST Webbook
ripol	1701.00		NIST Webbook
ripol	1717.00		NIST Webbook
ripol	1721.00		NIST Webbook
ripol	1740.00		NIST Webbook
ripol	1706.00		NIST Webbook
ripol	1731.00		NIST Webbook
tb	479.20	K	NIST Webbook

tb	480.25 ± 1.00	K	NIST Webbook
tb	480.00	K	NIST Webbook
tb	299.95 ± 0.40	K	NIST Webbook
tb	478.70 ± 0.50	K	NIST Webbook
tc	667.35	K	Joback Method
tf	292.98	K	Aqueous Solubility Prediction Method
tf	288.00	K	NIST Webbook
tf	296.00 ± 0.50	K	NIST Webbook
tf	295.65 ± 0.50	K	NIST Webbook
tf	295.65 ± 0.30	K	NIST Webbook
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.28	J/mol×K	458.94	Joback Method
cpg	244.14	J/mol×K	528.41	Joback Method
cpg	284.22	J/mol×K	667.35	Joback Method
cpg	254.88	J/mol×K	563.14	Joback Method
cpg	265.14	J/mol×K	597.88	Joback Method
cpg	274.92	J/mol×K	632.61	Joback Method
cpg	232.94	J/mol×K	493.67	Joback Method
dvisc	0.0002157	Pa×s	426.34	Joback Method
dvisc	0.0002771	Pa×s	393.73	Joback Method
dvisc	0.0003725	Pa×s	361.13	Joback Method
dvisc	0.0005310	Pa×s	328.53	Joback Method
dvisc	0.0008184	Pa×s	295.92	Joback Method
dvisc	0.0001740	Pa×s	458.94	Joback Method
dvisc	0.0014041	Pa×s	263.32	Joback Method
hvapt	52.70	kJ/mol	420.50	NIST Webbook
pvap	37.20	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	23.10	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	13.70	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
pvap	4.15	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	2.66	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	6.40	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	363.20	K	1.30	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Liquid-Liquid Equilibria of Formic Acid and Furfural in a Biphasic Aqueous-Organic System: Optimization of Solvent and Amine Extractant:	https://www.doi.org/10.1021/acs.jced.8b00335
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:	https://www.doi.org/10.1021/je0302349
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91167&Units=SI

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
hfus:	Enthalpy of fusion 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume