Benzoic acid, ethyl ester

Other names:	2-methoxy-1-phenyl-ethanone
	BENZOIC ETHER
	ETHYL BENZENECARBOXYLATE
	Essence of niobe
	Ethyl benzoate
	Ethylester kyseliny benzoove
Inchi:	InChI=1S/C9H10O2/c1-2-11-9(10)8-6-4-3-5-7-8/h3-7H,2H2,1H3
InchiKey:	MTZQAGJQAFMTAQ-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	CCOC(=O)c1ccccc1
Mol. weight [g/mol]:	150.17
CAS:	93-89-0

Physical Properties

Property code	Value	Unit	Source
af	0.4800		KDB
gf	-96.61	kJ/mol	Joback Method
hf	-237.36	kJ/mol	Joback Method
hfus	15.89	kJ/mol	Joback Method
hvap	61.10 ± 0.30	kJ/mol	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
log10ws	-2.32		Aqueous Solubility Prediction Method
log10ws	-2.32		Estimated Solubility Method
logp	1.863		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=1)		KDB
pc	3050.00	kPa	Critical Point Measurements for n-Alkyl Benzoates (C8 to C13)
pc	2320.00	kPa	KDB
rinpol	1141.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1164.00		NIST Webbook

rinpol	1178.00	NIST Webbook
rinpol	1157.00	NIST Webbook
rinpol	1142.00	NIST Webbook
rinpol	1133.38	NIST Webbook
rinpol	1154.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1151.00	NIST Webbook
rinpol	1146.00	NIST Webbook
rinpol	1170.00	NIST Webbook
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rinpol	1170.00	NIST Webbook
rinpol	1171.00	NIST Webbook
rinpol	1174.00	NIST Webbook
rinpol	1177.00	NIST Webbook
rinpol	1151.00	NIST Webbook
rinpol	1173.00	NIST Webbook
rinpol	1147.00	NIST Webbook
rinpol	1184.00	NIST Webbook
rinpol	1149.00	NIST Webbook
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rinpol	1147.00	NIST Webbook
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rinpol	1187.00	NIST Webbook
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rinpol	1133.38	NIST Webbook
rinpol	1153.14	NIST Webbook
rinpol	1148.70	NIST Webbook
rinpol	1144.00	NIST Webbook
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ripol	1651.00		NIST Webbook
ripol	1698.00		NIST Webbook
ripol	1663.00		NIST Webbook
ripol	1673.00		NIST Webbook
tb	484.95 ± 1.00	K	NIST Webbook
tb	482.30 ± 0.60	K	NIST Webbook
tb	485.70	K	KDB
tb	486.20	K	NIST Webbook
tb	486.00	K	NIST Webbook
tb	485.65 ± 0.40	K	NIST Webbook
tb	485.60 ± 0.30	K	NIST Webbook
tb	485.60 ± 0.50	K	NIST Webbook
tb	484.00 ± 4.00	K	NIST Webbook
tb	486.05 ± 0.40	K	NIST Webbook
tb	485.60 ± 0.50	K	NIST Webbook
tc	668.70	K	KDB
tf	238.30	K	KDB
tf	239.00	K	NIST Webbook
tf	238.40 ± 0.30	K	NIST Webbook
tf	238.45 ± 0.30	K	NIST Webbook
tf	238.60 ± 0.40	K	NIST Webbook
tf	240.90 ± 0.40	K	NIST Webbook
tf	238.95 ± 0.40	K	NIST Webbook
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.00	J/mol×K	544.32	Joback Method
cpg	321.72	J/mol×K	724.46	Joback Method
cpg	256.39	J/mol×K	508.29	Joback Method
cpg	312.50	J/mol×K	688.43	Joback Method
cpg	302.63	J/mol×K	652.40	Joback Method
cpg	280.90	J/mol×K	580.35	Joback Method

cpg	292.11	J/mol×K	616.37	Joback Method
cpl	246.00	J/mol×K	298.15	NIST Webbook
cpl	241.80	J/mol×K	292.70	NIST Webbook
cpl	241.80	J/mol×K	292.70	NIST Webbook
cpl	282.80	J/mol×K	290.00	NIST Webbook
dvisc	0.0014380	Pa×s	313.15	Viscosity, Density, and Refractive Index of Some (Ester + Hydrocarbon) Binary Mixtures at 303.15 K and 313.15 K
dvisc	0.0024440	Pa×s	288.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K
dvisc	0.0019710	Pa×s	298.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K
dvisc	0.0016240	Pa×s	308.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K

dvisc	0.0013680	Pa×s	318.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K
dvisc	0.0017480	Pa×s	303.15	Viscosity, Density, and Refractive Index of Some (Ester + Hydrocarbon) Binary Mixtures at 303.15 K and 313.15 K
hvapt	49.60 ± 0.20	kJ/mol	450.00	NIST Webbook
hvapt	46.70 ± 0.30	kJ/mol	450.00	NIST Webbook
hvapt	43.60 ± 0.50	kJ/mol	450.00	NIST Webbook
hvapt	57.00	kJ/mol	392.00	NIST Webbook
hvapt	50.50	kJ/mol	392.00	NIST Webbook
hvapt	55.90	kJ/mol	310.50	NIST Webbook
hvapt	50.40	kJ/mol	422.50	NIST Webbook
hvapt	51.90	kJ/mol	401.50	NIST Webbook
hvapt	52.50 ± 0.20	kJ/mol	450.00	NIST Webbook
pvap	0.13	kPa	320.30	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method

pvap	0.09	kPa	315.30	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method
pvap	0.07	kPa	312.30	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method
pvap	0.11	kPa	317.30	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method
pvap	0.17	kPa	323.40	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method

pvap	0.20	kPa	326.40	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method
pvap	0.25	kPa	329.50	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method
pvap	0.04	kPa	304.20	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method
pvap	7.10e-03	kPa	283.90	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method

pvap	9.30e-03	kPa	286.90	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method
pvap	0.01	kPa	289.00	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method
pvap	0.01	kPa	292.00	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method
pvap	0.29	kPa	332.50	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method

pvap	0.02	kPa	295.00	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method
pvap	0.02	kPa	298.10	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method
pvap	0.03	kPa	299.10	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method
pvap	0.03	kPa	301.20	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method

pvap	0.02	kPa	294.10	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method
pvap	0.05	kPa	307.20	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method
pvap	0.06	kPa	310.10	Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method
rhol	1041.42	kg/m3	298.15	Refractive Indices and Surface Tensions of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at (288.15, 298.15, 308.15, and 318.15) K

rhol	1041.30	kg/m3	298.15	Excess Molar Enthalpies for Dimethyl Carbonate with o-Xylene, m-Xylene, p-Xylene, Ethylbenzene or Ethyl Benzoate at 298.15 K and 10.2 MPa	
rhol	1041.30	kg/m3	298.15	Excess Molar Entalpies of Dimethyl Carbonate with o-Xylene, m-Xylene, p-Xylene, Ethylbenzene, or Ethyl Benzoate at 298.15 K	
rhol	1042.00	kg/m3	303.15	Study of molecular interactions in the mixtures of some primary alcohols with equimolar mixture of 1-propanol and alkylbenzoates at T = 303.15 K	
rhol	1046.00	kg/m3	293.00	KDB	
srf	0.03	N/m	308.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K	
srf	0.03	N/m	318.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K	
srf	0.03	N/m	298.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K	

srf	0.03	N/m	328.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	338.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	348.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.04	N/m	288.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	358.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	360.20	K	1.30	NIST Webbook
tbrp	360.30	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52741e+01
Coeff. B	-4.71347e+03
Coeff. C	-4.42100e+01
Temperature range (K), min.	358.72
Temperature range (K), max.	517.33

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.97631e+01
Coeff. B	-8.66976e+03
Coeff. C	-7.77947e+00
Coeff. D	3.43034e-06
Temperature range (K), min.	238.45
Temperature range (K), max.	698.00

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Limiting Diffusion Coefficients of Ethyl Benzoate, Benzylacetone, and Eugenol in Carbon Dioxide at Supercritical Conditions:	https://www.doi.org/10.1021/je700646e
Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K:	https://www.doi.org/10.1021/je050170x
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93890&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Cinnamate at 298.15 K:	https://www.doi.org/10.1021/je050389b
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1142
Excess Molar Enthalpies of Dimethyl Carbonate with Styrene, m-Xylene, p-Xylene, Ethylbenzene, or Ethyl Benzoate:	https://www.doi.org/10.1021/je020120h
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Thermodynamic Properties of Mixtures Containing Ionic Liquids. 7. Activity Coefficients of Aliphatic and Aromatic Esters and Benzylamine in 1-Methyl-3-ethylimidazolium Bis(trifluoromethylsulfonyl) Imide Using the Transpiration Method:	https://www.doi.org/10.1021/je050334+
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Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume