ETHYL BENZOATE

Other names:	2-methoxy-1-phenyl-ethanone
	Benzoic ether
	Essence of niobe
	Ethylester kyseliny benzoove
	benzoic acid, ethyl ester
	ethyl benzenecarboxylate
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]:	150.18
CAS:	93-89-0

Physical Properties

Property code	Value	Unit	Source
af	0.4800		KDB
gf	-96.61	kJ/mol	Joback Method
hf	-303.65	kJ/mol	Cheméo Relay (1.0)
hfus	15.89	kJ/mol	Joback Method
hvap	61.10 ± 0.30	kJ/mol	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
log10ws	-2.32		Estimated Solubility Method
log10ws	-2.32		Aqueous Solubility Prediction 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	1177.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1173.00		NIST Webbook

rinpol	1156.00	NIST Webbook
rinpol	1184.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1170.00	NIST Webbook
rinpol	1172.90	NIST Webbook
rinpol	1172.00	NIST Webbook
rinpol	1155.00	NIST Webbook
rinpol	1206.00	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
rinpol	1185.00	NIST Webbook
rinpol	1170.00	NIST Webbook
rinpol	1156.00	NIST Webbook
rinpol	1173.00	NIST Webbook
rinpol	1170.00	NIST Webbook
rinpol	1154.00	NIST Webbook
rinpol	1162.00	NIST Webbook
rinpol	1168.00	NIST Webbook
rinpol	1154.00	NIST Webbook
rinpol	1172.00	NIST Webbook
rinpol	1175.00	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
rinpol	1143.00	NIST Webbook
rinpol	1139.00	NIST Webbook
rinpol	1154.00	NIST Webbook
rinpol	1147.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1150.00	NIST Webbook
rinpol	1146.00	NIST Webbook
rinpol	1179.00	NIST Webbook
rinpol	1170.00	NIST Webbook
rinpol	1170.00	NIST Webbook
rinpol	1176.00	NIST Webbook
rinpol	1147.00	NIST Webbook

rinpol	1138.00	NIST Webbook
rinpol	1170.00	NIST Webbook
rinpol	1165.00	NIST Webbook
rinpol	1170.00	NIST Webbook
rinpol	1170.80	NIST Webbook
rinpol	1146.00	NIST Webbook
rinpol	1171.00	NIST Webbook
rinpol	1176.00	NIST Webbook
rinpol	1176.00	NIST Webbook
rinpol	1175.00	NIST Webbook
rinpol	1141.00	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1139.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1170.00	NIST Webbook
rinpol	1187.00	NIST Webbook
rinpol	1170.00	NIST Webbook
rinpol	1155.00	NIST Webbook
rinpol	1160.00	NIST Webbook
rinpol	1172.00	NIST Webbook
rinpol	1169.00	NIST Webbook
rinpol	1206.00	NIST Webbook
rinpol	1153.00	NIST Webbook
rinpol	1156.00	NIST Webbook
rinpol	1155.00	NIST Webbook
rinpol	1156.00	NIST Webbook
rinpol	1154.00	NIST Webbook
rinpol	1153.00	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1154.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1155.00	NIST Webbook
rinpol	1154.00	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1155.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1157.00	NIST Webbook
rinpol	1147.00	NIST Webbook
rinpol	1179.00	NIST Webbook
rinpol	1168.00	NIST Webbook
rinpol	1184.00	NIST Webbook
rinpol	1141.00	NIST Webbook
rinpol	1170.00	NIST Webbook

rinpol	1170.00	NIST Webbook
rinpol	1138.20	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1172.00	NIST Webbook
rinpol	1175.00	NIST Webbook
rinpol	1133.38	NIST Webbook
rinpol	1142.00	NIST Webbook
rinpol	1157.00	NIST Webbook
rinpol	1178.00	NIST Webbook
rinpol	1164.00	NIST Webbook
rinpol	1133.38	NIST Webbook
rinpol	1153.14	NIST Webbook
rinpol	1148.70	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	1142.00	NIST Webbook
rinpol	1174.00	NIST Webbook
rinpol	1147.00	NIST Webbook
rinpol	1169.00	NIST Webbook
rinpol	1166.00	NIST Webbook
rinpol	1157.00	NIST Webbook
rinpol	1176.00	NIST Webbook
rinpol	1164.00	NIST Webbook
rinpol	1176.00	NIST Webbook
rinpol	1179.00	NIST Webbook
rinpol	1178.00	NIST Webbook
rinpol	1160.00	NIST Webbook
rinpol	1171.00	NIST Webbook
rinpol	1152.00	NIST Webbook
rinpol	1157.00	NIST Webbook
rinpol	1164.00	NIST Webbook
rinpol	1160.00	NIST Webbook
rinpol	1160.00	NIST Webbook
rinpol	1175.00	NIST Webbook
rinpol	1172.90	NIST Webbook
rinpol	1171.00	NIST Webbook
rinpol	1149.00	NIST Webbook
rinpol	1154.00	NIST Webbook
rinpol	1172.00	NIST Webbook
rinpol	1180.00	NIST Webbook
rinpol	1171.00	NIST Webbook
rinpol	1168.00	NIST Webbook
rinpol	1173.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1173.00	NIST Webbook

rinpol	1170.00	NIST Webbook
rinpol	1171.00	NIST Webbook
rinpol	1170.00	NIST Webbook
rinpol	1170.00	NIST Webbook
rinpol	1141.00	NIST Webbook
ripol	1647.00	NIST Webbook
ripol	1709.00	NIST Webbook
ripol	1693.00	NIST Webbook
ripol	1689.00	NIST Webbook
ripol	1705.00	NIST Webbook
ripol	1658.00	NIST Webbook
ripol	1640.00	NIST Webbook
ripol	1641.00	NIST Webbook
ripol	1645.00	NIST Webbook
ripol	1653.00	NIST Webbook
ripol	1634.00	NIST Webbook
ripol	1644.00	NIST Webbook
ripol	1685.00	NIST Webbook
ripol	1640.00	NIST Webbook
ripol	1683.00	NIST Webbook
ripol	1685.00	NIST Webbook
ripol	1658.00	NIST Webbook
ripol	1653.00	NIST Webbook
ripol	1681.00	NIST Webbook
ripol	1670.00	NIST Webbook
ripol	1645.00	NIST Webbook
ripol	1663.00	NIST Webbook
ripol	1677.00	NIST Webbook
ripol	1684.00	NIST Webbook
ripol	1685.00	NIST Webbook
ripol	1681.00	NIST Webbook
ripol	1653.00	NIST Webbook
ripol	1673.00	NIST Webbook
ripol	1647.00	NIST Webbook
ripol	1658.00	NIST Webbook
ripol	1650.00	NIST Webbook
ripol	1694.00	NIST Webbook
ripol	1693.00	NIST Webbook
ripol	1694.00	NIST Webbook
ripol	1693.00	NIST Webbook
ripol	1656.00	NIST Webbook
ripol	1643.00	NIST Webbook
ripol	1670.00	NIST Webbook
ripol	1647.00	NIST Webbook

ripol	1650.00	NIST Webbook
ripol	1650.00	NIST Webbook
ripol	1662.00	NIST Webbook
ripol	1706.00	NIST Webbook
ripol	1662.00	NIST Webbook
ripol	1662.00	NIST Webbook
ripol	1649.00	NIST Webbook
ripol	1683.00	NIST Webbook
ripol	1666.00	NIST Webbook
ripol	1660.00	NIST Webbook
ripol	1660.00	NIST Webbook
ripol	1653.00	NIST Webbook
ripol	1663.00	NIST Webbook
ripol	1657.00	NIST Webbook
ripol	1647.00	NIST Webbook
ripol	1651.00	NIST Webbook
ripol	1645.00	NIST Webbook
ripol	1650.00	NIST Webbook
ripol	1653.00	NIST Webbook
ripol	1640.00	NIST Webbook
ripol	1680.00	NIST Webbook
ripol	1664.00	NIST Webbook
ripol	1678.00	NIST Webbook
ripol	1681.00	NIST Webbook
ripol	1706.00	NIST Webbook
ripol	1672.00	NIST Webbook
ripol	1681.00	NIST Webbook
ripol	1649.00	NIST Webbook
ripol	1670.00	NIST Webbook
ripol	1655.00	NIST Webbook
ripol	1668.00	NIST Webbook
ripol	1676.00	NIST Webbook
ripol	1654.00	NIST Webbook
ripol	1655.00	NIST Webbook
ripol	1651.00	NIST Webbook
ripol	1647.00	NIST Webbook
ripol	1650.00	NIST Webbook
ripol	1650.00	NIST Webbook
ripol	1650.00	NIST Webbook
ripol	1652.00	NIST Webbook
ripol	1653.00	NIST Webbook
ripol	1675.00	NIST Webbook
ripol	1651.00	NIST Webbook
ripol	1698.00	NIST Webbook

ripol	1673.00		NIST Webbook
ripol	1673.00		NIST Webbook
ripol	1649.00		NIST Webbook
ripol	1648.00		NIST Webbook
ripol	1644.00		NIST Webbook
ripol	1658.00		NIST Webbook
tb	485.60 ± 0.50	K	NIST Webbook
tb	486.20	K	NIST Webbook
tb	484.95 ± 1.00	K	NIST Webbook
tb	486.05 ± 0.40	K	NIST Webbook
tb	482.30 ± 0.60	K	NIST Webbook
tb	484.00 ± 4.00	K	NIST Webbook
tb	486.00	K	NIST Webbook
tb	485.60 ± 0.50	K	NIST Webbook
tb	485.60 ± 0.30	K	NIST Webbook
tb	485.65 ± 0.40	K	NIST Webbook
tb	485.70	K	KDB
tc	668.70	K	KDB
tf	238.60 ± 0.40	K	NIST Webbook
tf	238.30	K	KDB
tf	238.95 ± 0.40	K	NIST Webbook
tf	240.90 ± 0.40	K	NIST Webbook
tf	238.45 ± 0.30	K	NIST Webbook
tf	238.40 ± 0.30	K	NIST Webbook
tf	239.00	K	NIST Webbook
vc	0.447	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.39	J/mol×K	508.29	Joback Method
cpg	269.00	J/mol×K	544.32	Joback Method
cpg	280.90	J/mol×K	580.35	Joback Method
cpg	292.11	J/mol×K	616.37	Joback Method
cpg	302.63	J/mol×K	652.40	Joback Method
cpg	312.50	J/mol×K	688.43	Joback Method
cpg	321.72	J/mol×K	724.46	Joback Method
cpl	246.00	J/mol×K	298.15	NIST Webbook
cpl	282.80	J/mol×K	290.00	NIST Webbook
cpl	241.80	J/mol×K	292.70	NIST Webbook
cpl	241.80	J/mol×K	292.70	NIST Webbook

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	0.0016240	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	0.0017480	Pa×s	303.15	Viscosity, Density, and Refractive Index of Some (Ester + Hydrocarbon) Binary Mixtures at 303.15 K and 313.15 K	
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
hvapt	55.90	kJ/mol	310.50	NIST Webbook
hvapt	46.70 ± 0.30	kJ/mol	450.00	NIST Webbook
hvapt	51.90	kJ/mol	401.50	NIST Webbook
hvapt	50.40	kJ/mol	422.50	NIST Webbook
hvapt	43.60 ± 0.50	kJ/mol	450.00	NIST Webbook
hvapt	50.50	kJ/mol	392.00	NIST Webbook
hvapt	57.00	kJ/mol	392.00	NIST Webbook
hvapt	49.60 ± 0.20	kJ/mol	450.00	NIST Webbook
hvapt	52.50 ± 0.20	kJ/mol	450.00	NIST Webbook
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	0.13	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	0.03	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	0.06	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
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	0.09	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	0.11	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	0.03	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	0.02	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	0.02	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	0.17	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	0.29	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	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	0.04	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	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	0.02	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
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	1046.00	kg/m3	293.00	KDB
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
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	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	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	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	0.03	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

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1142

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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+

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Excess Molar Enthalpies of Dimethyl Carbonate with o-Xylene, m-Xylene, p-Xylene, Ethylbenzene, or Ethyl Benzoate at 298.15 K: https://www.doi.org/10.1021/je020120h

Study of molecular interactions in the mixtures of some primary alcohols with equimolar mixture of 1-propanol and alkylbenzoates at (298.15 K): https://www.doi.org/10.1016/j.jct.2013.09.005

Viscosity, Density, and Refractive Index of Some (Ester + Hydrocarbon) Binary Mixtures at 303.15 K and 313.15 K: https://www.doi.org/10.1021/je0400052

Viscosity, Density, and Refractive Index Data of Ethyl Benzoate, Benzylacetone, and Eugenol in Carbon Dioxide at Supercritical Conditions: https://www.doi.org/10.1021/je700646e

KDB: https://www.cheric.org/files/research/kdb/mol/mol1142.mol

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: https://www.doi.org/10.1021/je0601208

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C93890&Units=SI

Chemeo Relay (1.0):

Partition Coefficients of Organic Solutes between Supercritical Carbon Dioxide and Water: Experimental Measurements and Empirical Correlations: https://www.doi.org/10.1021/je030197l

Critical Point Measurements for n-Alkyl Benzoates (C8 to C12): https://www.doi.org/10.1021/je700049s

Effect of halogen substitution on the enthalpies of solvation and hydrogen bonding of organic solutes in ethylbenzene and 1,2-dichlorobenzene derived using the Kamlet–Taft solvatochromic equation: https://www.doi.org/10.1016/j.tca.2015.08.015

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: https://www.doi.org/10.1021/je020181f

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Examination of hydrogen-bonding interactions between dissolved solutes and alkylbenzene solvents based on Abraham model correlations: https://www.doi.org/10.1016/j.tca.2014.08.024

Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Pure Esters and Excess Properties of Their Binary Mixtures: https://www.doi.org/10.1021/je050170x

Abraham model correlations for solvent enthalpy of solvation and non-measured enthalpies of solvation: https://www.doi.org/10.1021/je050389b

UNIFAC - Magnussen (1981) - Revised and Extended Methods: http://link.springer.com/article/10.1007/BF02311772

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