Acetic acid, phenylmethyl ester

Other names:	(Acetoxymethyl)benzene
	ACETIC ACID PHENYLMETHYL ESTER
	Acetic acid, benzyl ester
	Benzyl acetate
	Benzyl ester of acetic acid
	Benzyl ethanoate
	Benzylester kyseliny octove
	NCI-C06508
	NSC 4550
	PHENYLMETHYL ACETATE
	Plastolin I
	ethanoic acid, benzyl ester
	ethanoic acid, phenylmethyl ester
	«alpha»-Acetoxytoluene
	Â«alphaÂ»-Acetoxytoluene
Inchi:	InChI=1S/C9H10O2/c1-8(10)11-7-9-5-3-2-4-6-9/h2-6H,7H2,1H3
InchiKey:	QUKGYYKBILRGFE-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	CC(=O)OCc1ccccc1
Mol. weight [g/mol]:	150.17
CAS:	140-11-4

Physical Properties

Property code	Value	Unit	Source
ea	0.15 ± 0.10	eV	NIST Webbook
gf	-96.61	kJ/mol	Joback Method
hf	-237.36	kJ/mol	Joback Method
hfus	15.89	kJ/mol	Joback Method
hvap	55.50	kJ/mol	NIST Webbook
log10ws	-2.05		Crippen Method
logp	1.750		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
rinpol	1137.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1144.00		NIST Webbook

rinpol	1144.00	NIST Webbook
rinpol	1136.00	NIST Webbook
rinpol	1134.00	NIST Webbook
rinpol	1123.00	NIST Webbook
rinpol	1133.00	NIST Webbook
rinpol	1161.00	NIST Webbook
rinpol	1163.00	NIST Webbook
rinpol	1169.10	NIST Webbook
rinpol	1162.00	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	1163.00	NIST Webbook
rinpol	1163.00	NIST Webbook
rinpol	1164.00	NIST Webbook
rinpol	1149.00	NIST Webbook
rinpol	1163.00	NIST Webbook
rinpol	1164.00	NIST Webbook
rinpol	1168.30	NIST Webbook
rinpol	1134.00	NIST Webbook
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rinpol	1171.00	NIST Webbook
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rinpol	1169.00	NIST Webbook
rinpol	1133.00	NIST Webbook
rinpol	1133.00	NIST Webbook
rinpol	1134.00	NIST Webbook
rinpol	1177.00	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1127.00	NIST Webbook
rinpol	1130.00	NIST Webbook
rinpol	1160.00	NIST Webbook
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rinpol	1160.00	NIST Webbook
rinpol	1170.00	NIST Webbook
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rinpol	1129.40	NIST Webbook
rinpol	1131.80	NIST Webbook
rinpol	1163.00	NIST Webbook
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ripol	1693.00		NIST Webbook
ripol	1695.00		NIST Webbook
ripol	1771.00		NIST Webbook
ripol	1747.00		NIST Webbook
ripol	1713.00		NIST Webbook
ripol	1710.00		NIST Webbook
ripol	1762.00		NIST Webbook
ripol	1741.00		NIST Webbook
tb	479.20	K	NIST Webbook
tb	486.25	K	Measurements of Quaternary Liquid-Liquid Equilibrium for Water + Acetic Acid + Propionic Acid + Solvent (Butyronitrile, Benzyl Acetate, or Methyl Isobutyl Ketone) at 298.15 K
tb	488.10 ± 0.50	K	NIST Webbook
tb	488.10 ± 0.50	K	NIST Webbook
tb	487.15 ± 0.50	K	NIST Webbook
tb	487.00	K	NIST Webbook
tc	724.46	K	Joback Method
tf	221.65 ± 0.30	K	NIST Webbook
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.39	J/mol×K	508.29	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

cpg	269.00	J/mol×K	544.32	Joback Method
cpl	250.20	J/mol×K	292.70	NIST Webbook
cpl	148.50	J/mol×K	298.15	NIST Webbook
cpl	250.20	J/mol×K	292.70	NIST Webbook
cpl	154.00	J/mol×K	306.00	NIST Webbook
dvisc	0.0025300	Pa×s	288.15	Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T) (288.15, 298.15, 308.15, and 318.15) K
dvisc	0.0020560	Pa×s	298.15	Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T) (288.15, 298.15, 308.15, and 318.15) K
dvisc	0.0017030	Pa×s	308.15	Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T) (288.15, 298.15, 308.15, and 318.15) K

dvisc	0.0014320	Pa×s	318.15	Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T) (288.15, 298.15, 308.15, and 318.15) K
hvapt	60.40	kJ/mol	305.50	NIST Webbook
rfi	1.49970		303.15	Excess Volumes of Binary Solutions of Methyl Formate, Ethyl Formate, Propyl Formate, and Benzyl Acetate with Bromo-, Chloro-, and Nitrobenzenes at (303.15, 308.15, and 313.15) K
rhol	1051.10	kg/m3	298.15	Thermodynamics of aromatic polar compound (alkanone, alkanal or alkanoate) + hydrocarbon mixtures
rhol	1051.10	kg/m3	298.15	Liquid Liquid Equilibria for Systems Containing 4-Phenylbutan-2-one or Benzyl Ethanoate and Selected Alkanes
rhol	1050.75	kg/m3	298.15	Refractive Indices and Surface Tensions of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at (288.15, 298.15, 308.15, and 318.15) 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	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	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	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	358.15	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	308.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.04	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	0.04	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	0.04	N/m	293.15	Densities, Viscosities, Refractive Indexes, and Surface Tensions for Mixtures of Ethanol, Benzyl Acetate, and Benzyl Alcohol
srf	0.04	N/m	303.15	Densities, Viscosities, Refractive Indexes, and Surface Tensions for Mixtures of Ethanol, Benzyl Acetate, and Benzyl Alcohol
srf	0.03	N/m	313.15	Densities, Viscosities, Refractive Indexes, and Surface Tensions for Mixtures of Ethanol, Benzyl Acetate, and Benzyl Alcohol
srf	0.03	N/m	323.15	Densities, Viscosities, Refractive Indexes, and Surface Tensions for Mixtures of Ethanol, Benzyl Acetate, and Benzyl Alcohol

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	407.00	K	13.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49623e+01
Coeff. B	-4.40919e+03
Coeff. C	-6.08920e+01
Temperature range (K), min.	361.35
Temperature range (K), max.	517.77

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.69268e+01
Coeff. B	-9.85763e+03
Coeff. C	-1.01888e+01
Coeff. D	4.04632e-06
Temperature range (K), min.	221.65
Temperature range (K), max.	699.00

Sources

Liquid Liquid Equilibria for Systems Containing 4-Phenylbutan-2-one or Benzyl Ethanoate and Selected Alkanes:	https://www.doi.org/10.1021/acs.jced.6b00803
Excess Volumes of Binary Solutions of Methyl Formate, Ethyl Formate, Propyl Formate, and Benzyl Acetate with Bromo-, Chloro-, and Nitrobenzenes at (303.15, 308.15, and 313.15) K:	https://www.doi.org/10.1021/je700150e
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1143.mol
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1143
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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility and Mass Transfer Coefficient Enhancement of Benzyl Acetate in Water through Hydrotropy:	https://www.doi.org/10.1021/je0342872
Measurements of Quaternary Liquid-Liquid Equilibrium for Water + Acetic Acid + Propionic Acid + Solvent (Butyronitrile, Benzyl Acetate, or Methyl Isobutyl Ketone) at 298.15 K:	https://www.doi.org/10.1021/je050527x
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T) (288.15, 298.15, 308.15, and 318.15) K:	https://www.doi.org/10.1021/je050402s
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C140114&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Thermodynamics of aromatic polar compound (alkanone, alkanal or alkanoate) + hydrocarbon mixtures:	https://www.doi.org/10.1016/j.fluid.2016.04.004

Refractive Indices and Surface Tensions of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at (288.15, 298.15, 308.15, and 318.15) K: https://www.doi.org/10.1021/je060139a

Densities, Viscosities, Refractive Indexes, and Surface Tensions for Mixtures of Ethanol + Benzyl Acetate and Benzyl Alcohol https://www.doi.org/10.1021/je201009c

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
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