Benzaldehyde

Other names:	Almond artificial essential oil
	Artifical essential oil of almond
	Artificial Almond Oil
	Artificial bitter almond oil
	Artificial essential oil of almond
	BENZENECARBONAL
	BENZENECARBOXALDEHYDE
	BENZOIC ALDEHYDE
	Benzaldehyde FFC
	Benzene carbaldehyde
	Benzenemethylal
	Benzoyl hydride
	Benzyaldehyde
	Benzylaldehyde
	Ethereal oil of bitter almonds
	NA 1989
	NCI-C56133
	NSC 7917
	Oil of Bitter Almond
	Phenylmethanal
	Phenylmethanal benzenecarboxaldehyde
Inchi:	InChI=1S/C7H6O/c8-6-7-4-2-1-3-5-7/h1-6H
InchiKey:	HUMNYLRZRPPJDN-UHFFFAOYSA-N
Formula:	C7H6O
SMILES:	O=Cc1ccccc1
Mol. weight [g/mol]:	106.12
CAS:	100-52-7

Physical Properties

Property code	Value	Unit	Source
af	0.3160		KDB
affp	834.00	kJ/mol	NIST Webbook
affp	831.70 ± 1.30	kJ/mol	NIST Webbook
aigt	465.37	K	KDB
basg	802.10	kJ/mol	NIST Webbook
basg	802.50 ± 3.40	kJ/mol	NIST Webbook

chl	-3526.00	kJ/mol	NIST Webbook
chl	-3529.00 ± 0.80	kJ/mol	NIST Webbook
chl	-3525.00 ± 2.00	kJ/mol	NIST Webbook
dm	2.80	debye	KDB
ea	0.43 ± 0.01	eV	NIST Webbook
ea	0.39 ± 0.05	eV	NIST Webbook
ea	0.42 ± 0.01	eV	NIST Webbook
ep	11.00	J/mol×K	NIST Webbook
fpc	347.04	K	KDB
fpo	337.59	K	KDB
gf	22.40	kJ/mol	KDB
hf	-37.00 ± 4.20	kJ/mol	NIST Webbook
hf	-37.20 ± 0.92	kJ/mol	NIST Webbook
hf	-40.40	kJ/mol	NIST Webbook
hf	-33.26	kJ/mol	NIST Webbook
hf	-36.80 ± 3.00	kJ/mol	NIST Webbook
hf	-36.80	kJ/mol	KDB
hfl	-87.10 ± 2.20	kJ/mol	NIST Webbook
hfl	-83.05 ± 0.84	kJ/mol	NIST Webbook
hfl	-86.20	kJ/mol	NIST Webbook
hfus	10.22	kJ/mol	Joback Method
hvap	40.17	kJ/mol	Joback Method
ie	9.60 ± 0.02	eV	NIST Webbook
ie	9.49	eV	NIST Webbook
ie	9.35	eV	NIST Webbook
ie	9.50 ± 0.08	eV	NIST Webbook
ie	9.74	eV	NIST Webbook
ie	9.50 ± 0.02	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	9.54	eV	NIST Webbook
ie	9.53 ± 0.03	eV	NIST Webbook
ie	9.57	eV	NIST Webbook
ie	9.71	eV	NIST Webbook
ie	9.49	eV	NIST Webbook
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ie	9.60	eV	NIST Webbook
ie	9.51 ± 0.02	eV	NIST Webbook
ie	9.65	eV	NIST Webbook
log10ws	-1.25		Aqueous Solubility Prediction Method
log10ws	-1.19		Estimated Solubility Method
logp	1.499		Crippen Method

mcvol	87.300	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=2)		KDB
pc	4650.00	kPa	KDB
pc	4410.00	kPa	Vapor-liquid critical point measurements of fifteen compounds by the pulse-heating method
pc	4650.00 ± 46.46	kPa	NIST Webbook
pc	2178.49 ± 303.98	kPa	NIST Webbook
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ripol	1488.00		NIST Webbook
ripol	1482.00		NIST Webbook
ripol	1509.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1520.00		NIST Webbook
ripol	1520.00		NIST Webbook
ripol	1520.00		NIST Webbook
ripol	1502.00		NIST Webbook
ripol	1502.00		NIST Webbook
ripol	1512.00		NIST Webbook
ripol	1486.00		NIST Webbook
ripol	1515.00		NIST Webbook
ripol	1494.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1527.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1520.00		NIST Webbook
ripol	1520.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1520.00		NIST Webbook
ripol	1470.00		NIST Webbook
sl	221.20	J/mol×K	NIST Webbook
tb	452.20	K	KDB
tc	695.00	K	KDB
tc	690.00 ± 20.00	K	NIST Webbook
tc	695.00 ± 5.00	K	NIST Webbook
tc	625.15 ± 3.00	K	NIST Webbook
tf	247.00	K	NIST Webbook
tf	259.70 ± 0.50	K	NIST Webbook
tf	216.25 ± 0.60	K	NIST Webbook
tf	217.55 ± 0.50	K	NIST Webbook
tf	216.65 ± 0.50	K	NIST Webbook
tf	247.00	K	KDB
tt	216.02 ± 0.02	K	NIST Webbook
vc	0.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.62	J/mol×K	617.26	Joback Method

cpg	155.23	J/mol×K	434.90	Joback Method
cpg	165.37	J/mol×K	471.37	Joback Method
cpg	174.84	J/mol×K	507.85	Joback Method
cpg	183.69	J/mol×K	544.32	Joback Method
cpg	191.94	J/mol×K	580.79	Joback Method
cpg	206.76	J/mol×K	653.74	Joback Method
cpl	172.00	J/mol×K	298.15	NIST Webbook
cpl	171.10	J/mol×K	302.30	NIST Webbook
cpl	171.10	J/mol×K	302.40	NIST Webbook
dvisc	0.0011306	Pa×s	313.15	Densities and Viscosities of (1-Propanol + 1,2-Dichloroethane), (1-Propanol + Benzaldehyde), (Benzaldehyde + 1,2-Dichloroethane), and (1-Propanol + 1,2-Dichloroethane + Benzaldehyde) Mixtures from T = 288.15 K to 313.15 K
dvisc	0.0012229	Pa×s	308.15	Densities and Viscosities of (1-Propanol + 1,2-Dichloroethane), (1-Propanol + Benzaldehyde), (Benzaldehyde + 1,2-Dichloroethane), and (1-Propanol + 1,2-Dichloroethane + Benzaldehyde) Mixtures from T = 288.15 K to 313.15 K
dvisc	0.0013155	Pa×s	303.15	Densities and Viscosities of (1-Propanol + 1,2-Dichloroethane), (1-Propanol + Benzaldehyde), (Benzaldehyde + 1,2-Dichloroethane), and (1-Propanol + 1,2-Dichloroethane + Benzaldehyde) Mixtures from T = 288.15 K to 313.15 K

dvisc	0.0014271	Pa×s	298.15	Densities and Viscosities of (1-Propanol + 1,2-Dichloroethane), (1-Propanol + Benzaldehyde), (Benzaldehyde + 1,2-Dichloroethane), and (1-Propanol + 1,2-Dichloroethane + Benzaldehyde) Mixtures from T = 288.15 K to 313.15 K
dvisc	0.0015581	Pa×s	293.15	Densities and Viscosities of (1-Propanol + 1,2-Dichloroethane), (1-Propanol + Benzaldehyde), (Benzaldehyde + 1,2-Dichloroethane), and (1-Propanol + 1,2-Dichloroethane + Benzaldehyde) Mixtures from T = 288.15 K to 313.15 K
dvisc	0.0017044	Pa×s	288.15	Densities and Viscosities of (1-Propanol + 1,2-Dichloroethane), (1-Propanol + Benzaldehyde), (Benzaldehyde + 1,2-Dichloroethane), and (1-Propanol + 1,2-Dichloroethane + Benzaldehyde) Mixtures from T = 288.15 K to 313.15 K
dvisc	0.0011200	Pa×s	318.15	Density and Viscosity of Acrylonitrile + Cinnamaldehyde, + Anisaldehyde, and + Benzaldehyde at (298.15, 308.15, and 318.15) K
dvisc	0.0012240	Pa×s	308.15	Density and Viscosity of Acrylonitrile + Cinnamaldehyde, + Anisaldehyde, and + Benzaldehyde at (298.15, 308.15, and 318.15) K

dvisc	0.0013990	Pa×s	298.15	Density and Viscosity of Acrylonitrile + Cinnamaldehyde, + Anisaldehyde, and + Benzaldehyde at (298.15, 308.15, and 318.15) K
hfust	9.32	kJ/mol	216.00	NIST Webbook
hfust	9.33	kJ/mol	216.00	NIST Webbook
hfust	9.32	kJ/mol	216.02	NIST Webbook
hvapt	50.30	kJ/mol	311.00	NIST Webbook
hvapt	42.50	kJ/mol	357.50	NIST Webbook
hvapt	47.00	kJ/mol	323.00	NIST Webbook
hvapt	40.60	kJ/mol	564.00	NIST Webbook
hvapt	41.90	kJ/mol	503.00	NIST Webbook
hvapt	45.50	kJ/mol	422.50	NIST Webbook
hvapt	48.60	kJ/mol	343.50	NIST Webbook
hvapt	54.40	kJ/mol	375.50	NIST Webbook
hvapt	43.80	kJ/mol	445.00	NIST Webbook
hvapt	49.50	kJ/mol	400.00	NIST Webbook
pvap	0.14	kPa	294.30	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furanaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol
pvap	0.43	kPa	313.20	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furanaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol
pvap	0.32	kPa	308.20	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furanaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol

pvap	0.25	kPa	303.20	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furanaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol	
pvap	10.00	kPa	377.63	Isobaric vapor-liquid equilibrium for binary system of cinnamaldehyde + benzaldehyde at 10, 20 and 30 kPa	
pvap	20.00	kPa	396.65	Isobaric vapor-liquid equilibrium for binary system of cinnamaldehyde + benzaldehyde at 10, 20 and 30 kPa	
pvap	30.00	kPa	408.67	Isobaric vapor-liquid equilibrium for binary system of cinnamaldehyde + benzaldehyde at 10, 20 and 30 kPa	
pvap	0.04	kPa	278.40	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furanaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol	
pvap	0.06	kPa	282.30	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furanaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol	

pvap	0.08	kPa	286.30	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furanaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol
pvap	0.10	kPa	290.30	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furanaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol
pvap	0.18	kPa	298.40	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furanaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol
rhol	1036.15	kg/m3	308.15	Densities and volumetric properties of binary mixtures of the ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate with benzaldehyde at T = (298.15 to 313.15) K
rhol	1019.10	kg/m3	323.15	Influence of Temperature and Carbon Chain on Thermophysical Properties of Benzaldehyde/Alkan-2-ol Binary Mixtures
rhol	1023.40	kg/m3	318.15	Influence of Temperature and Carbon Chain on Thermophysical Properties of Benzaldehyde/Alkan-2-ol Binary Mixtures

rhol	1046.30	kg/m3	293.15	Influence of Temperature and Carbon Chain on Thermophysical Properties of Benzaldehyde/Alkan-2-ol Binary Mixtures
rhol	1045.00	kg/m3	293.00	KDB
rhol	1027.90	kg/m3	313.15	Influence of Temperature and Carbon Chain on Thermophysical Properties of Benzaldehyde/Alkan-2-ol Binary Mixtures
rhol	1031.70	kg/m3	303.15	Density, Viscosity, Sound Speed, and Thermoacoustical Parameters of Benzaldehyde with Chlorobenzene or Nitrobenzene at 303.15 K, 308.15 K, and 313.15 K
rhol	1031.30	kg/m3	308.15	Density, Viscosity, Sound Speed, and Thermoacoustical Parameters of Benzaldehyde with Chlorobenzene or Nitrobenzene at 303.15 K, 308.15 K, and 313.15 K
rhol	1028.00	kg/m3	313.15	Density, Viscosity, Sound Speed, and Thermoacoustical Parameters of Benzaldehyde with Chlorobenzene or Nitrobenzene at 303.15 K, 308.15 K, and 313.15 K
rhol	1035.70	kg/m3	303.15	Density, Viscosity, Sound Speed, and Thermoacoustical Parameters of Benzaldehyde with Chlorobenzene or Nitrobenzene at 303.15 K, 308.15 K, and 313.15 K

rhol	1032.40	kg/m3	308.15	Influence of Temperature and Carbon Chain on Thermophysical Properties of Benzaldehyde/Alkan-2-ol Binary Mixtures
rhol	1043.61	kg/m3	298.15	Densities and excess volumes of binary mixtures of the ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate with aromatic compound at T = (298.15 to 313.15) K
rhol	1037.10	kg/m3	303.15	Influence of Temperature and Carbon Chain on Thermophysical Properties of Benzaldehyde/Alkan-2-ol Binary Mixtures
rhol	1041.70	kg/m3	298.15	Influence of Temperature and Carbon Chain on Thermophysical Properties of Benzaldehyde/Alkan-2-ol Binary Mixtures
rhol	1018.40	kg/m3	323.15	Thermophysical and optical studies of molecular interactions in binary mixtures of diethyl carbonate with aromatic compounds at temperatures from 298.15 to 323.15 K
rhol	1023.00	kg/m3	318.15	Thermophysical and optical studies of molecular interactions in binary mixtures of diethyl carbonate with aromatic compounds at temperatures from 298.15 to 323.15 K

rhol	1027.50	kg/m3	313.15	Thermophysical and optical studies of molecular interactions in binary mixtures of diethyl carbonate with aromatic compounds at temperatures from 298.15 to 323.15 K	
rhol	1032.00	kg/m3	308.15	Thermophysical and optical studies of molecular interactions in binary mixtures of diethyl carbonate with aromatic compounds at temperatures from 298.15 to 323.15 K	
rhol	1036.50	kg/m3	303.15	Thermophysical and optical studies of molecular interactions in binary mixtures of diethyl carbonate with aromatic compounds at temperatures from 298.15 to 323.15 K	
rhol	1042.94	kg/m3	298.15	Liquid-liquid equilibria for benzaldehyde + n-alkane mixtures andcharacterization of benzaldehyde + hydrocarbon systems in terms of DISQUAC	
rhol	1041.00	kg/m3	298.15	Thermophysical and optical studies of molecular interactions in binary mixtures of diethyl carbonate with aromatic compounds at temperatures from 298.15 to 323.15 K	

rhol	1040.21	kg/m3	303.15	Densities and volumetric properties of binary mixtures of the ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate with benzaldehyde at T = (298.15 to 313.15) K
rhol	1032.15	kg/m3	313.15	Densities and volumetric properties of binary mixtures of the ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate with benzaldehyde at T = (298.15 to 313.15) K
rhol	1044.20	kg/m3	298.15	Densities and volumetric properties of binary mixtures of the ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate with benzaldehyde at T = (298.15 to 313.15) K
sfust	43.14	J/mol×K	216.02	NIST Webbook
speedsl	1384.71	m/s	318.15	Volumetric and Acoustic Properties of Binary Mixtures of Cyclohexane + Benzene and + Benzaldehyde at (293.15 to 323.15) K
speedsl	1402.93	m/s	313.15	Volumetric and Acoustic Properties of Binary Mixtures of Cyclohexane + Benzene and + Benzaldehyde at (293.15 to 323.15) K
speedsl	1421.24	m/s	308.15	Volumetric and Acoustic Properties of Binary Mixtures of Cyclohexane + Benzene and + Benzaldehyde at (293.15 to 323.15) K

speedsl	1439.68	m/s	303.15	Volumetric and Acoustic Properties of Binary Mixtures of Cyclohexane + Benzene and + Benzaldehyde at (293.15 to 323.15) K
speedsl	1458.21	m/s	298.15	Volumetric and Acoustic Properties of Binary Mixtures of Cyclohexane + Benzene and + Benzaldehyde at (293.15 to 323.15) K
speedsl	1366.65	m/s	323.15	Volumetric and Acoustic Properties of Binary Mixtures of Cyclohexane + Benzene and + Benzaldehyde at (293.15 to 323.15) K
speedsl	1476.74	m/s	293.15	Volumetric and Acoustic Properties of Binary Mixtures of Cyclohexane + Benzene and + Benzaldehyde at (293.15 to 323.15) K

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	335.20	K	1.30	NIST Webbook
tbrp	452.00	K	100.00	NIST Webbook
tbrp	335.00	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.46798e+01
Coeff. B	-3.99219e+03
Coeff. C	-5.52190e+01
Temperature range (K), min.	332.61
Temperature range (K), max.	481.36

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.78778e+01
Coeff. B	-8.17952e+03
Coeff. C	-7.46624e+00
Coeff. D	2.42851e-06
Temperature range (K), min.	247.15
Temperature range (K), max.	695.00

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Influence of Temperature and Carbon Chain on Thermophysical Properties of Benzaldehyde/Alkan-2-ol Binary Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00335
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KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1245
Densities and volumetric properties of binary mixtures of the ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate with benzaldehyde at T = (298.15 to 318.15) K:	https://www.doi.org/10.1016/j.jct.2009.02.007
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Densities and excess volumes of binary mixtures of the ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate with aromatic compound at T = (298.15 to 318.15) K:	https://www.doi.org/10.1016/j.jct.2006.07.001
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Legend

af:	Acentric Factor
affp:	Proton affinity
aigt:	Autoignition Temperature
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
ea:	Electron affinity
ep:	Protonation entropy at 298K
fpc:	Flash Point (Closed Cup Method)
fpo:	Flash Point (Open Cup Method)
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume