Benzophenone

Other names:	1-Benzophenone
	ALPHA-OXODIPHENYLMETHANE
	Adjutan 6016
	Benzene, benzoyl-
	Benzoylbenzene
	Cinnarizine M (benzophenone)
	Cyclizine M (Benzophenone)
	DIPHENYL METHANONE
	Diphenyl ketone
	Diphenyl-methanon
	Diphenylmethanone
	Kayacure BP
	Ketone, diphenyl
	Methanone, diphenyl-
	NSC 8077
	PHENYL KETONE
	alpha-Oxoditane
	«alpha»-Oxodiphenylmethane
	«alpha»-Oxoditane
	Â«alphaÂ»-Oxodiphenylmethane
	Â«alphaÂ»-Oxoditane
Inchi:	InChI=1S/C13H10O/c14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10H
InchiKey:	RWCCWEUUXYIKHB-UHFFFAOYSA-N
Formula:	C13H10O
SMILES:	O=C(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	182.22
CAS:	119-61-9

Physical Properties

Property code	Value	Unit	Source
affp	882.30	kJ/mol	NIST Webbook
basg	852.50	kJ/mol	NIST Webbook
chs	-6498.00	kJ/mol	NIST Webbook
chs	-6512.00	kJ/mol	NIST Webbook
chs	-6512.40 ± 3.20	kJ/mol	NIST Webbook
chs	-6504.00	kJ/mol	NIST Webbook

chs	-6510.30 ± 2.10	kJ/mol	NIST Webbook
chs	-6510.00 ± 2.00	kJ/mol	NIST Webbook
ea	0.69 ± 0.05	eV	NIST Webbook
ea	1.11 ± 0.04	eV	NIST Webbook
ea	0.62 ± 0.10	eV	NIST Webbook
ea	0.66 ± 0.09	eV	NIST Webbook
ea	0.64 ± 0.05	eV	NIST Webbook
gf	154.48	kJ/mol	Joback Method
hf	49.90 ± 3.00	kJ/mol	NIST Webbook
hfs	-50.84	kJ/mol	NIST Webbook
hfs	-33.00	kJ/mol	NIST Webbook
hfs	-34.00	kJ/mol	NIST Webbook
hfs	-32.30 ± 3.30	kJ/mol	NIST Webbook
hfus	19.11	kJ/mol	Joback Method
hvap	94.98	kJ/mol	NIST Webbook
ie	9.08 ± 0.04	eV	NIST Webbook
ie	9.05 ± 0.05	eV	NIST Webbook
ie	9.50 ± 0.10	eV	NIST Webbook
ie	9.05	eV	NIST Webbook
ie	9.28	eV	NIST Webbook
ie	9.46	eV	NIST Webbook
ie	9.14 ± 0.03	eV	NIST Webbook
ie	9.46 ± 0.05	eV	NIST Webbook
ie	9.35 ± 0.04	eV	NIST Webbook
ie	9.40 ± 0.10	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.50 ± 0.10	eV	NIST Webbook
log10ws	-3.12		Estimated Solubility Method
log10ws	-3.12		Aqueous Solubility Prediction Method
logp	2.918		Crippen Method
mcvol	148.080	ml/mol	McGowan Method
pc	3352.00 ± 4.00	kPa	NIST Webbook
rhoc	321.07 ± 3.64	kg/m3	NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1635.10		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1573.00		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1577.00		NIST Webbook

rinpol	1612.00	NIST Webbook
rinpol	1636.00	NIST Webbook
rinpol	1572.00	NIST Webbook
rinpol	1610.00	NIST Webbook
rinpol	1610.00	NIST Webbook
rinpol	1640.00	NIST Webbook
rinpol	1627.00	NIST Webbook
rinpol	1645.00	NIST Webbook
rinpol	1628.00	NIST Webbook
rinpol	1612.00	NIST Webbook
rinpol	1635.00	NIST Webbook
rinpol	1644.00	NIST Webbook
rinpol	1604.00	NIST Webbook
rinpol	1655.00	NIST Webbook
rinpol	1590.00	NIST Webbook
rinpol	1594.00	NIST Webbook
rinpol	1603.00	NIST Webbook
rinpol	1603.00	NIST Webbook
rinpol	1610.00	NIST Webbook
rinpol	1610.00	NIST Webbook
rinpol	1623.00	NIST Webbook
rinpol	1611.00	NIST Webbook
rinpol	1621.00	NIST Webbook
rinpol	1610.40	NIST Webbook
rinpol	1644.00	NIST Webbook
rinpol	1644.00	NIST Webbook
rinpol	1621.00	NIST Webbook
rinpol	1621.00	NIST Webbook
rinpol	1611.00	NIST Webbook
rinpol	1664.00	NIST Webbook
rinpol	1606.40	NIST Webbook
rinpol	1631.00	NIST Webbook
rinpol	1634.00	NIST Webbook
rinpol	1585.00	NIST Webbook
rinpol	1612.00	NIST Webbook
rinpol	1625.00	NIST Webbook
ripol	2457.00	NIST Webbook
ripol	2410.00	NIST Webbook
ripol	2470.00	NIST Webbook
ripol	2462.00	NIST Webbook
ripol	2505.00	NIST Webbook
ripol	2427.00	NIST Webbook
ripol	2443.00	NIST Webbook
ripol	2427.00	NIST Webbook

tb	578.97	K	KDB
tc	830.00 ± 2.00	K	NIST Webbook
tf	321.43	K	Aqueous Solubility Prediction Method
tf	321.15	K	KDB
tt	321.03 ± 0.02	K	NIST Webbook
tt	323.40	K	Determination of Solubility and Thermodynamic Properties of Benzophenone in Different Pure Solvents
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.27	J/mol×K	604.07	Joback Method
cpg	406.11	J/mol×K	814.39	Joback Method
cpg	395.61	J/mol×K	772.32	Joback Method
cpg	384.06	J/mol×K	730.26	Joback Method
cpg	371.37	J/mol×K	688.20	Joback Method
cpg	357.47	J/mol×K	646.13	Joback Method
cpg	415.64	J/mol×K	856.45	Joback Method
cpl	301.80	J/mol×K	325.00	Application of fast scanning calorimetry to the fusion thermochemistry of low-molecular-weight organic compounds: Fast-crystallizing m-terphenyl heat capacities in a deeply supercooled liquid state

cpl	274.50	J/mol×K	265.00	Application of fast scanning calorimetry to the fusion thermochemistry of low-molecular-weight organic compounds: Fast-crystallizing m-terphenyl heat capacities in a deeply supercooled liquid state
cpl	311.00	J/mol×K	345.00	Application of fast scanning calorimetry to the fusion thermochemistry of low-molecular-weight organic compounds: Fast-crystallizing m-terphenyl heat capacities in a deeply supercooled liquid state
cpl	265.30	J/mol×K	245.00	Application of fast scanning calorimetry to the fusion thermochemistry of low-molecular-weight organic compounds: Fast-crystallizing m-terphenyl heat capacities in a deeply supercooled liquid state
cpl	269.90	J/mol×K	255.00	Application of fast scanning calorimetry to the fusion thermochemistry of low-molecular-weight organic compounds: Fast-crystallizing m-terphenyl heat capacities in a deeply supercooled liquid state

cpl	306.40	J/mol×K	335.00	Application of fast scanning calorimetry to the fusion thermochemistry of low-molecular-weight organic compounds: Fast-crystallizing m-terphenyl heat capacities in a deeply supercooled liquid state
cpl	279.00	J/mol×K	275.00	Application of fast scanning calorimetry to the fusion thermochemistry of low-molecular-weight organic compounds: Fast-crystallizing m-terphenyl heat capacities in a deeply supercooled liquid state
cpl	283.60	J/mol×K	285.00	Application of fast scanning calorimetry to the fusion thermochemistry of low-molecular-weight organic compounds: Fast-crystallizing m-terphenyl heat capacities in a deeply supercooled liquid state
cpl	288.10	J/mol×K	295.00	Application of fast scanning calorimetry to the fusion thermochemistry of low-molecular-weight organic compounds: Fast-crystallizing m-terphenyl heat capacities in a deeply supercooled liquid state

cpl	292.70	J/mol×K	305.00	Application of fast scanning calorimetry to the fusion thermochemistry of low-molecular-weight organic compounds: Fast-crystallizing m-terphenyl heat capacities in a deeply supercooled liquid state
cpl	297.30	J/mol×K	315.00	Application of fast scanning calorimetry to the fusion thermochemistry of low-molecular-weight organic compounds: Fast-crystallizing m-terphenyl heat capacities in a deeply supercooled liquid state
cps	224.80	J/mol×K	300.00	NIST Webbook
dvisc	0.0002631	Pa×s	559.90	Joback Method
dvisc	0.0002067	Pa×s	604.07	Joback Method
dvisc	0.0007319	Pa×s	427.38	Joback Method
dvisc	0.0012047	Pa×s	383.21	Joback Method
dvisc	0.0022577	Pa×s	339.04	Joback Method
dvisc	0.0003490	Pa×s	515.73	Joback Method
dvisc	0.0004882	Pa×s	471.55	Joback Method
hfust	18.47	kJ/mol	321.30	NIST Webbook
hfust	18.19	kJ/mol	324.20	NIST Webbook
hfust	17.67	kJ/mol	321.20	NIST Webbook
hfust	18.19	kJ/mol	321.00	NIST Webbook
hfust	18.19	kJ/mol	321.03	NIST Webbook
hfust	18.81	kJ/mol	222.50	NIST Webbook
hsubt	95.00 ± 1.50	kJ/mol	305.50	NIST Webbook
hsubt	96.10	kJ/mol	306.00	NIST Webbook
hsubt	95.00 ± 0.20	kJ/mol	304.00	NIST Webbook
hsubt	78.20 ± 1.20	kJ/mol	302.50	NIST Webbook
hsubt	95.00 ± 1.00	kJ/mol	321.00	NIST Webbook
hsubt	89.96	kJ/mol	308.00	NIST Webbook
hsubt	93.90 ± 0.50	kJ/mol	307.00	NIST Webbook
hsubt	78.20 ± 0.80	kJ/mol	313.00	NIST Webbook
hsubt	92.90 ± 0.80	kJ/mol	306.00	NIST Webbook
hvapt	65.10	kJ/mol	553.00	NIST Webbook

hvapt	62.20	kJ/mol	526.00	NIST Webbook
hvapt	59.00	kJ/mol	552.50	NIST Webbook
psub	9.39e-04	kPa	317.73	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
psub	1.24e-03	kPa	320.23	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
psub	1.19e-04	kPa	300.37	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
psub	1.61e-04	kPa	302.88	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
psub	7.08e-04	kPa	315.24	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
psub	4.01e-04	kPa	310.26	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
psub	3.02e-04	kPa	307.90	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
psub	2.20e-04	kPa	305.39	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation

psub	5.35e-04	kPa	312.75	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
sfust	55.00	J/mol×K	321.20	NIST Webbook
sfust	56.67	J/mol×K	321.03	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	497.00	K	13.30	NIST Webbook
tbrp	430.70	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56649e+01
Coeff. B	-5.82958e+03
Coeff. C	-5.04230e+01
Temperature range (K), min.	429.53
Temperature range (K), max.	613.48

Sources

Application of fast scanning calorimetry to the fusion thermochemistry of low-molecular-weight organic compounds. Fast-crystallizing m-terphenyl heat capacities in a deeply supercooled liquid state:	https://www.doi.org/10.1016/j.tca.2018.08.015
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1215.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119619&Units=SI

Determination of Solubility and Thermodynamic Properties of Benzophenone in Different Pure Solvents:	https://www.doi.org/10.1021/acs.jced.8b00196
Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation:	https://www.doi.org/10.1016/j.fluid.2014.11.026
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Solubility of Benzophenone in Binary Alkane + Carbon Tetrachloride Solvent Mixtures:	https://www.doi.org/10.1021/je0340497

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation 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
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor pressure
rhoc:	Critical density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
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