Biphenyl

Other names:	1,1'-Biphenyl
	1,1'-Diphenyl
	1,1-Biphenyl
	Bibenzene
	Carolid AL
	Diphenyl
	Lemonene
	NSC 14916
	PhPh
	Phenador-X
	Phenylbenzene
	Tetrosin LY
	Xenene
Inchi:	InChI=1S/C12H10/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1-10H
InchiKey:	ZUOUZKKEUPVFJK-UHFFFAOYSA-N
Formula:	C12H10
SMILES:	c1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	154.21
CAS:	92-52-4

Physical Properties

Property code	Value	Unit	Source
af	0.3720		KDB
affp	813.60	kJ/mol	NIST Webbook
affp	808.80	kJ/mol	NIST Webbook
basg	780.70	kJ/mol	NIST Webbook
basg	782.90	kJ/mol	NIST Webbook
ea	0.13 ± 0.04	eV	NIST Webbook
gf	280.30	kJ/mol	KDB
hf	182.20	kJ/mol	KDB
hfs	96.80 ± 4.00	kJ/mol	NIST Webbook
hfs	98.20 ± 2.50	kJ/mol	NIST Webbook
hfs	96.70 ± 2.60	kJ/mol	NIST Webbook
hfs	100.50 ± 1.50	kJ/mol	NIST Webbook
hfs	97.20 ± 1.60	kJ/mol	NIST Webbook

hfus	19.30	kJ/mol	Synthesis and characterization of novel binary organic monotectic and eutectic alloys
hvap	46.86	kJ/mol	Joback Method
ie	7.95 ± 0.02	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.16 ± 0.13	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	8.35	eV	NIST Webbook
ie	8.64	eV	NIST Webbook
ie	8.27 ± 0.01	eV	NIST Webbook
ie	8.22 ± 0.15	eV	NIST Webbook
ie	8.20 ± 0.05	eV	NIST Webbook
ie	8.46	eV	NIST Webbook
ie	8.23 ± 0.01	eV	NIST Webbook
ie	8.39	eV	NIST Webbook
ie	8.34	eV	NIST Webbook
ie	8.80 ± 0.05	eV	NIST Webbook
log10ws	-4.34		Estimated Solubility Method
log10ws	-4.38		Aqueous Solubility Prediction Method
logp	3.354		Crippen Method
mcvol	132.420	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=2)		KDB
pc	3218.08 ± 81.06	kPa	NIST Webbook
pc	3346.00 ± 103.42	kPa	NIST Webbook
pc	3500.00 ± 101.33	kPa	NIST Webbook
pc	3800.00 ± 689.50	kPa	NIST Webbook
pc	3226.19 ± 81.06	kPa	NIST Webbook
pc	3400.00 ± 100.00	kPa	NIST Webbook
pc	4084.00 ± 137.89	kPa	NIST Webbook
pc	3120.00 ± 202.65	kPa	NIST Webbook
pc	3380.00	kPa	KDB
rhoc	306.87 ± 14.96	kg/m3	NIST Webbook
rhoc	322.29 ± 10.02	kg/m3	NIST Webbook
rhoc	309.96 ± 10.02	kg/m3	NIST Webbook
rhoc	308.42 ± 15.42	kg/m3	NIST Webbook
rinpol	1351.00		NIST Webbook
rinpol	1354.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1349.00		NIST Webbook
rinpol	1350.00		NIST Webbook

rinpol	1389.00	NIST Webbook
rinpol	1377.30	NIST Webbook
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rinpol	1338.40	NIST Webbook
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rinpol	1396.81	NIST Webbook
rinpol	1392.00	NIST Webbook
rinpol	1392.64	NIST Webbook
rinpol	1390.72	NIST Webbook
rinpol	1384.00	NIST Webbook
rinpol	1374.00	NIST Webbook
rinpol	1378.00	NIST Webbook
rinpol	1349.00	NIST Webbook
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rinpol	1364.00	NIST Webbook
rinpol	1373.00	NIST Webbook
rinpol	1362.00	NIST Webbook
rinpol	1397.00	NIST Webbook
rinpol	1371.00	NIST Webbook
rinpol	1375.00	NIST Webbook
rinpol	1366.00	NIST Webbook
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rinpol	1360.00	NIST Webbook
rinpol	1408.00	NIST Webbook
rinpol	1368.00	NIST Webbook
rinpol	1396.00	NIST Webbook
rinpol	1384.00	NIST Webbook
rinpol	1385.30	NIST Webbook
rinpol	1379.00	NIST Webbook
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rinpol	1380.00	NIST Webbook

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rinpol	1349.00	NIST Webbook
rinpol	1350.00	NIST Webbook
rinpol	1389.00	NIST Webbook
rinpol	1389.00	NIST Webbook
rinpol	1399.00	NIST Webbook
rinpol	237.70	NIST Webbook
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rinpol	236.87	NIST Webbook

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rinpol	234.05	NIST Webbook
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rinpol	236.39	NIST Webbook
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rinpol	240.35	NIST Webbook
rinpol	229.33	NIST Webbook
rinpol	235.00	NIST Webbook
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rinpol	233.96	NIST Webbook
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rinpol	237.30	NIST Webbook
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rinpol	236.40	NIST Webbook
rinpol	232.86	NIST Webbook
rinpol	232.96	NIST Webbook

rinpol	236.20	NIST Webbook
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rinpol	1369.00	NIST Webbook
rinpol	233.96	NIST Webbook
rinpol	245.80	NIST Webbook
rinpol	1352.00	NIST Webbook
ripol	2016.00	NIST Webbook
ripol	2029.00	NIST Webbook
ripol	1996.00	NIST Webbook
ripol	1996.00	NIST Webbook
ripol	2012.00	NIST Webbook

ripol	2029.00		NIST Webbook
ripol	228.73		NIST Webbook
ripol	1981.00		NIST Webbook
ripol	1974.00		NIST Webbook
ripol	1974.00		NIST Webbook
ripol	1981.00		NIST Webbook
ripol	2012.00		NIST Webbook
ripol	1967.00		NIST Webbook
ripol	1981.00		NIST Webbook
ripol	2030.00		NIST Webbook
ss	209.38	J/mol×K	NIST Webbook
ss	209.00	J/mol×K	NIST Webbook
ss	205.90	J/mol×K	NIST Webbook
tb	529.20	K	KDB
tc	773.00	K	KDB
tc	769.00 ± 3.00	K	NIST Webbook
tc	789.00 ± 5.60	K	NIST Webbook
tc	777.00 ± 6.00	K	NIST Webbook
tc	773.00 ± 3.00	K	NIST Webbook
tc	773.00 ± 3.00	K	NIST Webbook
tc	800.00 ± 11.11	K	NIST Webbook
tc	768.75 ± 2.00	K	NIST Webbook
tf	342.10	K	The use of organic calibration standards in the enthalpy calibration of differential scanning calorimeters
tf	342.08	K	Investigation of the melting behavior of the reference materials biphenyl and phenyl salicylate by a new type adiabatic scanning calorimeter
tf	342.00	K	KDB
tf	342.84	K	Aqueous Solubility Prediction Method
tf	341.10	K	Solid-liquid equilibria of eicosane, tetracosane or biphenyl + 1- octadecanol, or + 1-eicosanol mixtures
tt	342.09 ± 0.01	K	NIST Webbook
tt	341.80 ± 0.30	K	NIST Webbook
vc	0.497	m3/kmol	KDB
vc	0.497	m3/kmol	NIST Webbook
zc	0.2613710		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.58	J/mol×K	777.19	Joback Method
cpg	294.98	J/mol×K	568.96	Joback Method
cpg	310.02	J/mol×K	610.61	Joback Method
cpg	323.82	J/mol×K	652.25	Joback Method
cpg	336.46	J/mol×K	693.90	Joback Method
cpg	348.02	J/mol×K	735.54	Joback Method
cpg	278.63	J/mol×K	527.32	Joback Method
cpl	263.20	J/mol×K	350.80	NIST Webbook
cpl	285.30	J/mol×K	370.00	NIST Webbook
cpl	301.20	J/mol×K	422.00	NIST Webbook
cpl	300.00	J/mol×K	370.00	NIST Webbook
cpl	259.54	J/mol×K	298.00	NIST Webbook
cps	194.10	J/mol×K	294.40	NIST Webbook
cps	198.39	J/mol×K	298.15	NIST Webbook
cps	197.70	J/mol×K	298.15	NIST Webbook
cps	190.00	J/mol×K	300.00	NIST Webbook
cps	190.80	J/mol×K	298.15	NIST Webbook
cps	197.90	J/mol×K	298.10	NIST Webbook
cps	197.90	J/mol×K	303.00	NIST Webbook
cps	198.17	J/mol×K	298.15	NIST Webbook
dvisc	0.0026453	Pa×s	277.84	Joback Method
dvisc	0.0013056	Pa×s	319.42	Joback Method
dvisc	0.0002032	Pa×s	527.32	Joback Method
dvisc	0.0002595	Pa×s	485.74	Joback Method
dvisc	0.0003470	Pa×s	444.16	Joback Method
dvisc	0.0007582	Pa×s	361.00	Joback Method
dvisc	0.0004926	Pa×s	402.58	Joback Method
hfust	18.66	kJ/mol	341.50	NIST Webbook
hfust	18.65	kJ/mol	341.50	NIST Webbook
hfust	19.27	kJ/mol	344.34	NIST Webbook
hfust	18.80	kJ/mol	344.10	NIST Webbook
hfust	19.70	kJ/mol	342.30	NIST Webbook
hfust	18.66	kJ/mol	341.50	NIST Webbook
hfust	18.58	kJ/mol	342.10	NIST Webbook
hfust	18.95	kJ/mol	314.30	NIST Webbook
hfust	18.59	kJ/mol	342.00	NIST Webbook
hfust	18.57	kJ/mol	343.00	NIST Webbook
hfust	18.58	kJ/mol	342.20	NIST Webbook
hsubt	81.52	kJ/mol	298.15	NIST Webbook

hsubt	68.60 ± 0.80	kJ/mol	295.00	NIST Webbook
hsubt	81.80	kJ/mol	383.00	NIST Webbook
hsubt	83.40	kJ/mol	310.50	NIST Webbook
hsubt	80.40 ± 1.60	kJ/mol	319.00	NIST Webbook
hsubt	75.20	kJ/mol	308.00	NIST Webbook
hsubt	83.60 ± 2.50	kJ/mol	283.00	NIST Webbook
hsubt	75.80 ± 0.60	kJ/mol	289.00	NIST Webbook
hsubt	81.60 ± 1.70	kJ/mol	301.00	NIST Webbook
hsubt	81.59	kJ/mol	288.05	NIST Webbook
hsubt	75.10 ± 1.70	kJ/mol	297.00	NIST Webbook
hsubt	68.60 ± 0.80	kJ/mol	292.00	NIST Webbook
hsubt	75.81 ± 0.59	kJ/mol	342.50	NIST Webbook
hsubt	76.00 ± 4.00	kJ/mol	293.00	NIST Webbook
hvapt	64.95	kJ/mol	298.00	Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects
hvapt	60.30	kJ/mol	464.00	NIST Webbook
hvapt	59.60	kJ/mol	400.50	NIST Webbook
hvapt	60.40	kJ/mol	363.00	NIST Webbook
hvapt	57.30	kJ/mol	476.50	NIST Webbook
hvapt	54.90	kJ/mol	416.50	NIST Webbook
hvapt	48.00	kJ/mol	647.00	NIST Webbook
hvapt	59.40	kJ/mol	443.00	NIST Webbook
hvapt	45.61	kJ/mol	528.20	KDB
hvapt	57.40	kJ/mol	464.00	NIST Webbook
hvapt	51.20	kJ/mol	591.50	NIST Webbook
hvapt	50.40	kJ/mol	464.00	NIST Webbook
pvap	0.12	kPa	347.70	Benchmark properties of biphenyl as a liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	0.57	kPa	376.20	Benchmark properties of biphenyl as a liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.54	kPa	375.40	Benchmark properties of biphenyl as a liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.48	kPa	373.10	Benchmark properties of biphenyl as a liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.37	kPa	368.20	Benchmark properties of biphenyl as a liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.16	kPa	353.30	Benchmark properties of biphenyl as a liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods	

pvap	0.28	kPa	363.30	Benchmark properties of biphenyl as a liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.22	kPa	358.30	Benchmark properties of biphenyl as a liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.10	kPa	345.70	Benchmark properties of biphenyl as a liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.14	kPa	350.40	Benchmark properties of biphenyl as a liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.12	kPa	348.30	Benchmark properties of biphenyl as a liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	0.35	kPa	368.20	Benchmark properties of biphenyl as a liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods
rhol	990.00	kg/m3	347.00	KDB
sfust	60.30	J/mol×K	314.30	NIST Webbook
sfust	54.40	J/mol×K	342.00	NIST Webbook
sfust	54.20	J/mol×K	343.00	NIST Webbook
sfust	54.81	J/mol×K	341.50	NIST Webbook
sfust	54.60	J/mol×K	341.50	NIST Webbook
sfust	54.60	J/mol×K	344.10	NIST Webbook
sfust	54.30	J/mol×K	342.20	NIST Webbook
sfust	54.30	J/mol×K	342.10	NIST Webbook
srf	0.03	N/m	393.20	KDB
ssubt	273.42	J/mol×K	298.15	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	418.20	K	2.90	NIST Webbook
tbrp	418.00	K	2.90	NIST Webbook
tbrp	347.00 ± 4.00	K	0.03	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.40474e+01
Coeff. B	-1.07952e+04
Coeff. C	-1.11711e+01
Coeff. D	3.86310e-06
Temperature range (K), min.	342.00
Temperature range (K), max.	789.26

Datasets

Specific volume, m3/kg

Temperature, K - Liquid	Pressure, kPa - Liquid	Specific volume, m3/kg - Liquid
333.15	100.00	0.0010
343.15	100.00	0.0010
353.15	100.00	0.0010
353.15	10000.00	0.0010
353.15	20000.00	0.0010
353.15	30000.00	0.0010
363.15	100.00	0.0010
363.16	100.00	0.0010
363.16	10000.00	0.0010
363.16	20000.00	0.0010
363.16	30000.00	0.0010
363.16	40000.00	0.0010
363.16	50000.00	0.0010
363.16	60000.00	0.0010
363.16	70000.00	0.0010

Reference *https://www.doi.org/10.1007/s10765-009-0625-z*

Sources

High-pressure phase diagram of the drug mitotane in compressed and/or supercritical CO2:	https://www.doi.org/10.1016/j.jct.2009.08.017
The use of organic calibration standards in the enthalpy calibration of differential scanning calorimeters:	https://www.doi.org/10.1016/j.tca.2012.03.028
Benchmark properties of biphenyl as a liquid organic hydrogen carrier:	https://www.doi.org/10.1016/j.jct.2018.02.025
Solid liquid gas equilibrium of the naphthalene biphenyl CO2 system:	https://www.doi.org/10.1016/j.fluid.2010.09.006
Evaluation of thermochemical data with complementary experimental and computational methods:	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92524&Units=SI
Solid-liquid equilibria of eicosane, tetracosane or biphenyl + 1-octadecanol, or + 1-eicosanol mixtures:	https://www.doi.org/10.1016/j.fluid.2017.03.012
Synthesis and characterization of novel binary organic monotectic and eutectic alloys:	https://www.doi.org/10.1016/j.tca.2012.02.020
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=767
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubilities of 4-Phenyltoluene, Phenylboric Acid, Biphenyl, and Iodobenzene in Carbon Dioxide from 313.15 to 393.15 K and Pressures up to 27.6 MPa:	https://www.doi.org/10.1021/je050075o
PVT Relationships of Binary Mixtures of Indole with 2-Methylnaphthalene and Biphenyl at Temperatures and Pressures up to 120 MPa:	https://www.doi.org/10.1007/s10765-009-0625-z
Measurements of the Relative Permittivity of Inorganic Salts on the Aqueous Solubility of Selected Chlorobenzenes:	https://www.doi.org/10.1021/je034170d
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=767
Thermophysical properties of diphenyl ether + biphenyl mixtures for their use as heat transfer fluids:	https://www.doi.org/10.1016/j.jct.2012.02.001
Investigation of the melting behavior of the reference materials biphenyl and phenyl salicylate by a new type adiabatic scanning calorimeter:	https://www.doi.org/10.1016/j.tca.2014.02.023
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=767
Isobaric heat capacity at high pressure, density, and viscosity of (diphenyl ether + biphenyl) mixtures:	https://www.doi.org/10.1016/j.jct.2015.09.028
Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects:	https://www.doi.org/10.1021/je800091s

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density

rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
srf:	Surface Tension
ss:	Solid phase molar entropy at standard conditions
ssubt:	Entropy of sublimation 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
vols:	Specific Volume
zc:	Critical Compressibility
zra:	Rackett Parameter