1,1'-Bicyclohexyl

Other names:	1,1'-Biphenyl, dodecahydro- 1,1-Bicyclohexyl BICYCLOHEXANE Bicyclohexyl Cyclohexane, cyclohexyl- Cyclohexylcyclohexane DICYCLOHEXYL DODECAHYDRO-1,1-BIPHENYL Dicyclohexane Dodecahydrobiphenyl NSC 59855
Inchi:	InChI=1S/C12H22/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h11-12H,1-10H2
InchiKey:	WVIIMZNLDWSIRH-UHFFFAOYSA-N
Formula:	C12H22
SMILES:	C1CCC(C2CCCCC2)CC1
Mol. weight [g/mol]:	166.30
CAS:	92-51-3

Physical Properties

Property code	Value	Unit	Source
chl	-7537.50 ± 6.30	kJ/mol	NIST Webbook
chl	-7596.50	kJ/mol	NIST Webbook
chl	-7439.65	kJ/mol	NIST Webbook
chl	-7589.90 ± 2.60	kJ/mol	NIST Webbook
chl	-7593.00 ± 1.00	kJ/mol	NIST Webbook
gf	99.06	kJ/mol	Joback Method
hf	-218.40 ± 3.10	kJ/mol	NIST Webbook
hf	-215.30	kJ/mol	NIST Webbook
hfl	-276.40 ± 3.10	kJ/mol	NIST Webbook
hfl	-273.30 ± 1.20	kJ/mol	NIST Webbook
hfus	10.51	kJ/mol	Joback Method
hvap	58.00 ± 0.20	kJ/mol	NIST Webbook
hvap	58.00	kJ/mol	NIST Webbook
hvap	58.00 ± 0.30	kJ/mol	NIST Webbook
hvap	57.98	kJ/mol	NIST Webbook
ie	9.41	eV	NIST Webbook
log10ws	-4.15		Crippen Method

logp	4.147		Crippen Method
mcvol	158.220	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	1313.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1301.20		NIST Webbook
rinpol	1293.10		NIST Webbook
rinpol	1301.50		NIST Webbook
rinpol	1307.80		NIST Webbook
rinpol	1304.39		NIST Webbook
rinpol	1293.10		NIST Webbook
rinpol	1301.50		NIST Webbook
rinpol	1307.80		NIST Webbook
rinpol	1301.50		NIST Webbook
rinpol	1301.20		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1313.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1301.50		NIST Webbook
ripol	1420.00		NIST Webbook
ripol	1431.00		NIST Webbook
tb	513.06	K	Joback Method
tc	745.11	K	Joback Method
tf	239.76	K	Joback Method
tt	276.90 ± 0.00	K	NIST Webbook
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.05	J/mol×K	513.06	Joback Method
cpg	518.21	J/mol×K	745.11	Joback Method
cpg	499.72	J/mol×K	706.43	Joback Method
cpg	479.81	J/mol×K	667.76	Joback Method
cpg	435.56	J/mol×K	590.41	Joback Method

cpg	458.45	J/mol×K	629.08	Joback Method
cpg	411.12	J/mol×K	551.73	Joback Method
cpl	300.40	J/mol×K	311.00	NIST Webbook
cpl	300.00	J/mol×K	313.00	NIST Webbook
cpl	283.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0003514	Pa×s	467.51	Joback Method
dvisc	0.0002550	Pa×s	513.06	Joback Method
dvisc	0.0035294	Pa×s	285.31	Joback Method
dvisc	0.0008424	Pa×s	376.41	Joback Method
dvisc	0.0108669	Pa×s	239.76	Joback Method
dvisc	0.0005190	Pa×s	421.96	Joback Method
dvisc	0.0015623	Pa×s	330.86	Joback Method
hfust	0.74	kJ/mol	267.50	NIST Webbook
hfust	6.86	kJ/mol	223.00	NIST Webbook
hfust	6.78	kJ/mol	277.20	NIST Webbook
hfust	1.54	kJ/mol	256.10	NIST Webbook
hfust	7.08	kJ/mol	273.50	NIST Webbook
hfust	6.78	kJ/mol	277.20	NIST Webbook
hvapt	42.50	kJ/mol	525.00	NIST Webbook
hvapt	50.10	kJ/mol	435.00	NIST Webbook
hvapt	53.80	kJ/mol	421.00	NIST Webbook
rfi	1.47870		293.15	Density, Viscosity, Refractive Index, and Freezing Point for Binary Mixtures of 1,1'-Bicyclohexyl with Alkylcyclohexane
rhol	871.74	kg/m3	313.15	Density and Viscosity from 293.15 to 373.15 K, Speed of Sound and Bulk Modulus from 293.15 to 343.15 K, Surface Tension, and Flash Point of Binary Mixtures of Bicyclohexyl and 1,2,3,4-Tetrahydronaphthalene or Trans-decahydronaphthalene at 0.1 MPa

rhol	864.58	kg/m3	323.15	Density and Viscosity from 293.15 to 373.15 K, Speed of Sound and Bulk Modulus from 293.15 to 343.15 K, Surface Tension, and Flash Point of Binary Mixtures of Bicyclohexyl and 1,2,3,4-Tetrahydronaphthalene or Trans-decahydronaphthalene at 0.1 MPa
rhol	857.43	kg/m3	333.15	Density and Viscosity from 293.15 to 373.15 K, Speed of Sound and Bulk Modulus from 293.15 to 343.15 K, Surface Tension, and Flash Point of Binary Mixtures of Bicyclohexyl and 1,2,3,4-Tetrahydronaphthalene or Trans-decahydronaphthalene at 0.1 MPa
rhol	878.93	kg/m3	303.15	Density and Viscosity from 293.15 to 373.15 K, Speed of Sound and Bulk Modulus from 293.15 to 343.15 K, Surface Tension, and Flash Point of Binary Mixtures of Bicyclohexyl and 1,2,3,4-Tetrahydronaphthalene or Trans-decahydronaphthalene at 0.1 MPa

rhol	843.00	kg/m3	353.15	Density and Viscosity from 293.15 to 373.15 K, Speed of Sound and Bulk Modulus from 293.15 to 343.15 K, Surface Tension, and Flash Point of Binary Mixtures of Bicyclohexyl and 1,2,3,4-Tetrahydronaphthalene or Trans-decahydronaphthalene at 0.1 MPa
rhol	835.90	kg/m3	363.15	Density and Viscosity from 293.15 to 373.15 K, Speed of Sound and Bulk Modulus from 293.15 to 343.15 K, Surface Tension, and Flash Point of Binary Mixtures of Bicyclohexyl and 1,2,3,4-Tetrahydronaphthalene or Trans-decahydronaphthalene at 0.1 MPa
rhol	886.13	kg/m3	293.15	Density and Viscosity from 293.15 to 373.15 K, Speed of Sound and Bulk Modulus from 293.15 to 343.15 K, Surface Tension, and Flash Point of Binary Mixtures of Bicyclohexyl and 1,2,3,4-Tetrahydronaphthalene or Trans-decahydronaphthalene at 0.1 MPa
rhol	886.05	kg/m3	293.15	Densities and Viscosities of Ternary System n-Dodecane (1) + Bicyclohexyl (2) + n-Butanol (3) and Corresponding Binaries at T = (293.15 to 333.15) K

rhol	882.44	kg/m3	298.15	Densities and Viscosities of Ternary System n-Dodecane (1) + Bicyclohexyl (2) + n-Butanol (3) and Corresponding Binaries at T = (293.15 to 333.15) K
rhol	878.84	kg/m3	303.15	Densities and Viscosities of Ternary System n-Dodecane (1) + Bicyclohexyl (2) + n-Butanol (3) and Corresponding Binaries at T = (293.15 to 333.15) K
rhol	875.25	kg/m3	308.15	Densities and Viscosities of Ternary System n-Dodecane (1) + Bicyclohexyl (2) + n-Butanol (3) and Corresponding Binaries at T = (293.15 to 333.15) K
rhol	871.66	kg/m3	313.15	Densities and Viscosities of Ternary System n-Dodecane (1) + Bicyclohexyl (2) + n-Butanol (3) and Corresponding Binaries at T = (293.15 to 333.15) K
rhol	868.08	kg/m3	318.15	Densities and Viscosities of Ternary System n-Dodecane (1) + Bicyclohexyl (2) + n-Butanol (3) and Corresponding Binaries at T = (293.15 to 333.15) K
rhol	864.50	kg/m3	323.15	Densities and Viscosities of Ternary System n-Dodecane (1) + Bicyclohexyl (2) + n-Butanol (3) and Corresponding Binaries at T = (293.15 to 333.15) K

rhol	860.93	kg/m3	328.15	Densities and Viscosities of Ternary System n-Dodecane (1) + Bicyclohexyl (2) + n-Butanol (3) and Corresponding Binaries at T = (293.15 to 333.15) K
rhol	850.29	kg/m3	343.15	Density and Viscosity from 293.15 to 373.15 K, Speed of Sound and Bulk Modulus from 293.15 to 343.15 K, Surface Tension, and Flash Point of Binary Mixtures of Bicyclohexyl and 1,2,3,4-Tetrahydronaphthalene or Trans-decahydronaphthalene at 0.1 MPa
rhol	828.60	kg/m3	373.15	Density and Viscosity from 293.15 to 373.15 K, Speed of Sound and Bulk Modulus from 293.15 to 343.15 K, Surface Tension, and Flash Point of Binary Mixtures of Bicyclohexyl and 1,2,3,4-Tetrahydronaphthalene or Trans-decahydronaphthalene at 0.1 MPa
rhol	857.35	kg/m3	333.15	Densities and Viscosities of Ternary System n-Dodecane (1) + Bicyclohexyl (2) + n-Butanol (3) and Corresponding Binaries at T = (293.15 to 333.15) K
sfust	25.89	J/mol×K	273.50	NIST Webbook
sfust	24.46	J/mol×K	277.20	NIST Webbook
sfust	6.01	J/mol×K	256.10	NIST Webbook
sfust	2.77	J/mol×K	267.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	372.50 ± 0.50	K	1.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50496e+01
Coeff. B	-4.73244e+03
Coeff. C	-5.43230e+01
Temperature range (K), min.	374.91
Temperature range (K), max.	540.29

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.73446e+01
Coeff. B	-1.02483e+04
Coeff. C	-1.18827e+01
Coeff. D	5.45803e-06
Temperature range (K), min.	276.78
Temperature range (K), max.	727.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92513&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=591
Density and Viscosity from 293.15 to 373.15 K, Speed of Sound and Bulk Modulus from 293.15 to 343.15 K, Surface Tension, and Flash Point of Binary Mixtures of Bicyclohexyl and 1,2,3,4-Tetrahydronaphthalene or Trans-decahydronaphthalene at 0.1 MPa:	https://www.doi.org/10.1021/acs.jced.5b00790
KDB:	https://www.cheric.org/files/research/kdb/mol/mol591.mol
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Density, Viscosity, Refractive Index, and Freezing Point for Binary Mixtures of 1,1′-Bicyclohexyl with Alkylcyclohexane:	https://www.doi.org/10.1021/je500275j
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Densities and Viscosities of Ternary System n-Dodecane (1) + Bicyclohexyl (2) + n-Butanol (3) and Corresponding Binaries at T = (293.15 to 333.15) K:	https://www.doi.org/10.1021/acs.jced.8b00438
Joback Method	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
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
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
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid 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