Benzene, cyclohexyl-

Other names:	1,1'-Biphenyl, 1,2,3,4,5,6-hexahydro-
	1,2,3,4,5,6-HEXAHYDRO-1,1'-BIPHENYL
	Cyclohexane, phenyl-
	Cyclohexylbenzene
	PHENYL CYCLOHEXANE
	Phenylcyclohexane
Inchi:	InChI=1S/C12H16/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1,3-4,7-8,12H,2,5-6,9-10H2
InchiKey:	IGARGHRYKHJQSM-UHFFFAOYSA-N
Formula:	C12H16
SMILES:	c1ccc(C2CCCCC2)cc1
Mol. weight [g/mol]:	160.26
CAS:	827-52-1

Physical Properties

Property code	Value	Unit	Source
chl	-6932.22 ± 0.92	kJ/mol	NIST Webbook
chl	-6929.60 ± 5.40	kJ/mol	NIST Webbook
gf	187.02	kJ/mol	Joback Method
hf	-16.70 ± 1.50	kJ/mol	NIST Webbook
hf	-14.20	kJ/mol	NIST Webbook
hfl	-76.60 ± 1.10	kJ/mol	NIST Webbook
hfl	-79.10 ± 5.60	kJ/mol	NIST Webbook
hfus	12.71	kJ/mol	Joback Method
hvap	45.01	kJ/mol	Joback Method
ie	8.10	eV	NIST Webbook
log10ws	-3.81		Crippen Method
logp	3.734		Crippen Method
mcvol	145.320	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
rinpol	1317.70		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1308.90		NIST Webbook
rinpol	1357.00		NIST Webbook

rinpol	1326.00		NIST Webbook
rinpol	1308.90		NIST Webbook
rinpol	1317.70		NIST Webbook
rinpol	1322.90		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1314.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1289.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1322.90		NIST Webbook
ripol	1661.00		NIST Webbook
ripol	1643.00		NIST Webbook
ripol	1660.00		NIST Webbook
ripol	1662.00		NIST Webbook
tb	513.27 ± 0.50	K	NIST Webbook
tb	513.27 ± 0.20	K	NIST Webbook
tb	508.70	K	NIST Webbook
tb	512.70	K	NIST Webbook
tc	760.98	K	Joback Method
tf	258.80	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.99	J/mol×K	760.98	Joback Method
cpg	374.06	J/mol×K	600.45	Joback Method
cpg	392.51	J/mol×K	640.58	Joback Method
cpg	409.61	J/mol×K	680.72	Joback Method
cpg	425.41	J/mol×K	720.85	Joback Method
cpg	354.19	J/mol×K	560.32	Joback Method
cpg	332.83	J/mol×K	520.19	Joback Method
cpl	263.20	J/mol×K	198.15	NIST Webbook
dvisc	0.0002271	Pa×s	520.19	Joback Method
dvisc	0.0004213	Pa×s	433.06	Joback Method
dvisc	0.0006366	Pa×s	389.50	Joback Method
dvisc	0.0010673	Pa×s	345.93	Joback Method
dvisc	0.0020766	Pa×s	302.37	Joback Method
dvisc	0.0003007	Pa×s	476.62	Joback Method

dvisc	0.0050551	Pa×s	258.80	Joback Method
hfust	15.30	kJ/mol	280.50	NIST Webbook
hfust	15.30	kJ/mol	280.50	NIST Webbook
hfust	15.27	kJ/mol	280.50	NIST Webbook
hvapt	51.30	kJ/mol	467.00	NIST Webbook
hvapt	56.40	kJ/mol	338.00	NIST Webbook
sfust	54.44	J/mol×K	280.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	400.70	K	4.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57050e+01
Coeff. B	-4.49734e+03
Coeff. C	-8.86800e+01
Temperature range (K), min.	380.39
Temperature range (K), max.	521.39

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.08191e+02
Coeff. B	-1.15507e+04
Coeff. C	-1.31757e+01
Coeff. D	4.30979e-06
Temperature range (K), min.	280.14
Temperature range (K), max.	744.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol749.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C827521&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=749

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
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
vc:	Critical Volume