Dodecylcyclohexane

Other names:	Cyclohexane, dodecyl- N-DODECYLCYCLOHEXANE dodecane, 1-cyclohexyl- n-Dodecyl cyclohexane
Inchi:	InChI=1S/C18H36/c1-2-3-4-5-6-7-8-9-10-12-15-18-16-13-11-14-17-18/h18H,2-17H2,1H3
InchiKey:	BLRBGKYYWDBAQQ-UHFFFAOYSA-N
Formula:	C18H36
SMILES:	CCCCCCCCCCCCC1CCCCC1
Mol. weight [g/mol]:	252.48
CAS:	1795-17-1

Physical Properties

Property code	Value	Unit	Source
chl	-11850.30 ± 2.60	kJ/mol	NIST Webbook
chl	-11760.60 ± 3.50	kJ/mol	NIST Webbook
gf	125.13	kJ/mol	Joback Method
hf	-378.10 ± 2.80	kJ/mol	NIST Webbook
hfl	-467.60 ± 3.60	kJ/mol	NIST Webbook
hfus	34.21	kJ/mol	Joback Method
hvap	93.40 ± 1.30	kJ/mol	NIST Webbook
hvap	89.50	kJ/mol	NIST Webbook
hvap	88.90 ± 0.80	kJ/mol	NIST Webbook
hvap	88.91 ± 0.96	kJ/mol	NIST Webbook
log10ws	-7.01		Crippen Method
logp	6.878		Crippen Method
mcvol	253.620	ml/mol	McGowan Method
pc	1331.01	kPa	Joback Method
rinpol	1864.00		NIST Webbook
rinpol	1864.00		NIST Webbook
rinpol	1822.00		NIST Webbook
rinpol	1818.00		NIST Webbook
tb	588.00 ± 4.00	K	NIST Webbook
tc	811.32	K	Joback Method
tf	285.00 ± 1.50	K	NIST Webbook
tf	282.30 ± 2.00	K	NIST Webbook
tt	285.80 ± 0.20	K	NIST Webbook
vc	0.977	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.95	J/mol×K	660.88	Joback Method
cpg	764.80	J/mol×K	690.97	Joback Method
cpg	785.58	J/mol×K	721.06	Joback Method
cpg	805.31	J/mol×K	751.15	Joback Method
cpg	824.03	J/mol×K	781.23	Joback Method
cpg	841.78	J/mol×K	811.32	Joback Method
cpg	719.98	J/mol×K	630.79	Joback Method
cpl	615.50	J/mol×K	298.15	NIST Webbook
dvisc	0.0004343	Pa×s	465.39	Joback Method
dvisc	0.0008032	Pa×s	410.26	Joback Method
dvisc	0.0002675	Pa×s	520.53	Joback Method
dvisc	0.0054127	Pa×s	300.00	Joback Method
dvisc	0.0001808	Pa×s	575.66	Joback Method
dvisc	0.0001308	Pa×s	630.79	Joback Method
dvisc	0.0017981	Pa×s	355.13	Joback Method
hfust	45.84	kJ/mol	258.80	NIST Webbook
hfust	45.84	kJ/mol	258.80	NIST Webbook
hfust	45.84	kJ/mol	258.80	NIST Webbook
hvapt	93.40	kJ/mol	311.50	NIST Webbook
rhol	822.31	kg/m3	293.15	Densities, Speeds of Sound, and Viscosities of Binary Mixtures of an n-Alkylcyclohexane (n-Propyl-, n-Pentyl-, n-Hexyl-, n-Heptyl, n-Octyl-, n-Nonyl-, n-Decyl-, and n-Dodecyl-) with n-Hexadecane
rhol	795.75	kg/m3	333.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations

rhol	802.38	kg/m3	323.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	809.03	kg/m3	313.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	815.68	kg/m3	303.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	819.02	kg/m3	298.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	825.71	kg/m3	288.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations

rhol	822.36	kg/m3	293.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	769.20	kg/m3	373.15	Densities, Speeds of Sound, and Viscosities of Binary Mixtures of an n-Alkylcyclohexane (n-Propyl-, n-Pentyl-, n-Hexyl-, n-Heptyl, n-Octyl-, n-Nonyl-, n-Decyl-, and n-Dodecyl-) with n-Hexadecane
rhol	775.90	kg/m3	363.15	Densities, Speeds of Sound, and Viscosities of Binary Mixtures of an n-Alkylcyclohexane (n-Propyl-, n-Pentyl-, n-Hexyl-, n-Heptyl, n-Octyl-, n-Nonyl-, n-Decyl-, and n-Dodecyl-) with n-Hexadecane
rhol	782.50	kg/m3	353.15	Densities, Speeds of Sound, and Viscosities of Binary Mixtures of an n-Alkylcyclohexane (n-Propyl-, n-Pentyl-, n-Hexyl-, n-Heptyl, n-Octyl-, n-Nonyl-, n-Decyl-, and n-Dodecyl-) with n-Hexadecane

rhol	789.10	kg/m3	343.15	Densities, Speeds of Sound, and Viscosities of Binary Mixtures of an n-Alkylcyclohexane (n-Propyl-, n-Pentyl-, n-Hexyl-, n-Heptyl, n-Octyl-, n-Nonyl-, n-Decyl-, and n-Dodecyl-) with n-Hexadecane
rhol	795.74	kg/m3	333.15	Densities, Speeds of Sound, and Viscosities of Binary Mixtures of an n-Alkylcyclohexane (n-Propyl-, n-Pentyl-, n-Hexyl-, n-Heptyl, n-Octyl-, n-Nonyl-, n-Decyl-, and n-Dodecyl-) with n-Hexadecane
rhol	802.37	kg/m3	323.15	Densities, Speeds of Sound, and Viscosities of Binary Mixtures of an n-Alkylcyclohexane (n-Propyl-, n-Pentyl-, n-Hexyl-, n-Heptyl, n-Octyl-, n-Nonyl-, n-Decyl-, and n-Dodecyl-) with n-Hexadecane
rhol	809.01	kg/m3	313.15	Densities, Speeds of Sound, and Viscosities of Binary Mixtures of an n-Alkylcyclohexane (n-Propyl-, n-Pentyl-, n-Hexyl-, n-Heptyl, n-Octyl-, n-Nonyl-, n-Decyl-, and n-Dodecyl-) with n-Hexadecane

rhol	815.65	kg/m3	303.15	Densities, Speeds of Sound, and Viscosities of Binary Mixtures of an n-Alkylcyclohexane (n-Propyl-, n-Pentyl-, n-Hexyl-, n-Heptyl, n-Octyl-, n-Nonyl-, n-Decyl-, and n-Dodecyl-) with n-Hexadecane
sfust	160.40	J/mol×K	258.80	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tfp	285.80	K	100.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	290.60	K	19500.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	295.20	K	39600.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	299.90	K	60900.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	304.20	K	79900.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	308.40	K	100000.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53949e+01
Coeff. B	-5.09043e+03
Coeff. C	-1.15638e+02
Temperature range (K), min.	452.59
Temperature range (K), max.	620.47

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.12957e+02
Coeff. B	-1.90387e+04
Coeff. C	-2.83025e+01
Coeff. D	1.22589e-05
Temperature range (K), min.	301.15
Temperature range (K), max.	657.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1795171&Units=SI
Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurement and Molecular Dynamics Simulations.	https://www.doi.org/10.1021/acs.jced.8b01135
Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes.	https://www.doi.org/10.1021/je600575r
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=601
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Densities, Speeds of Sound, and Viscosities of Binary Mixtures of an n-Alkylcyclohexane (n-Propyl-, n-Pentyl-, n-Hexyl-, n-Heptyl, n-Octyl-, n-Nonyl-, n-Decyl-, and n-Dodecyl-) with n-Hexadecane:	https://www.doi.org/10.1021/acs.jced.8b00692
KDB:	https://www.cheric.org/files/research/kdb/mol/mol601.mol
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tfp:	Melting point
tt:	Triple Point Temperature
vc:	Critical Volume