Heptylcyclohexane

Other names:	1-Cyclohexylheptane Cyclohexane, heptyl- Cyclohexane, n-heptyl- Heptane, 1-cyclohexyl- n-Heptyl cyclohexane n-heptylcyclohexane
Inchi:	InChI=1S/C13H26/c1-2-3-4-5-7-10-13-11-8-6-9-12-13/h13H,2-12H2,1H3
InchiKey:	MSTLSCNJAHAQNU-UHFFFAOYSA-N
Formula:	C13H26
SMILES:	CCCCCCCC1CCCCC1
Mol. weight [g/mol]:	182.35
CAS:	5617-41-4

Physical Properties

Property code	Value	Unit	Source
chl	-8556.60 ± 1.80	kJ/mol	NIST Webbook
chl	-8478.50 ± 2.30	kJ/mol	NIST Webbook
gf	83.03	kJ/mol	Joback Method
hf	-275.00 ± 1.90	kJ/mol	NIST Webbook
hfl	-353.00 ± 2.30	kJ/mol	NIST Webbook
hfus	21.26	kJ/mol	Joback Method
hvap	63.72 ± 0.54	kJ/mol	NIST Webbook
hvap	64.90	kJ/mol	NIST Webbook
log10ws	-4.92		Crippen Method
logp	4.927		Crippen Method
mcvol	183.170	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinpol	1341.77		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1349.58		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1341.77		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1343.00		NIST Webbook
rinpol	1343.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1328.00		NIST Webbook

rinpol	1335.38		NIST Webbook
rinpol	1339.99		NIST Webbook
rinpol	1342.75		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1346.47		NIST Webbook
sl	446.90	J/mol×K	NIST Webbook
tb	510.00 ± 4.00	K	NIST Webbook
tc	706.34	K	Joback Method
tf	232.00 ± 1.50	K	NIST Webbook
tt	232.80 ± 0.20	K	NIST Webbook
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.48	J/mol×K	516.39	Joback Method
cpg	487.34	J/mol×K	579.71	Joback Method
cpg	506.76	J/mol×K	611.37	Joback Method
cpg	525.21	J/mol×K	643.03	Joback Method
cpg	542.72	J/mol×K	674.68	Joback Method
cpg	559.32	J/mol×K	706.34	Joback Method
cpg	466.93	J/mol×K	548.05	Joback Method
cpl	363.20	J/mol×K	298.15	NIST Webbook
dvisc	0.0012433	Pa×s	334.56	Joback Method
dvisc	0.0006871	Pa×s	380.02	Joback Method
dvisc	0.0079072	Pa×s	243.65	Joback Method
dvisc	0.0004310	Pa×s	425.48	Joback Method
dvisc	0.0002958	Pa×s	470.93	Joback Method
dvisc	0.0002170	Pa×s	516.39	Joback Method
dvisc	0.0027110	Pa×s	289.11	Joback Method
hfust	22.22	kJ/mol	232.80	NIST Webbook
hfust	22.22	kJ/mol	232.80	NIST Webbook
hfust	22.23	kJ/mol	232.80	NIST Webbook

rhol	810.99	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	803.98	kg/m3	303.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	807.49	kg/m3	298.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	814.51	kg/m3	288.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	782.85	kg/m3	333.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations

rhol	789.91	kg/m3	323.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	796.95	kg/m3	313.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	803.99	kg/m3	303.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	811.00	kg/m3	293.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhol	754.40	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	761.60	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	768.70	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	775.80	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	782.83	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	789.89	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	796.93	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	803.96	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	95.50	J/mol×K	232.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48678e+01

Coeff. B	-4.31770e+03
Coeff. C	-8.87370e+01
Temperature range (K), min.	384.87
Temperature range (K), max.	540.56

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5617414&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations:	https://www.doi.org/10.1021/acs.jced.8b01135

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
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
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume