

Cyclohexane, pentyl-

Other names:	1-Cyclohexylpentane Amylcyclohexane Cyclohexane, n-pentyl- Pentane, 1-cyclohexyl- Pentylcyclohexane n-Amyl cyclohexane n-Pentylcyclohexane
Inchi:	InChI=1S/C11H22/c1-2-3-5-8-11-9-6-4-7-10-11/h11H,2-10H2,1H3
InchiKey:	HLTMUYBTNSVOFY-UHFFFAOYSA-N
Formula:	C11H22
SMILES:	CCCCC1CCCCC1
Mol. weight [g/mol]:	154.29
CAS:	4292-92-6

Physical Properties

Property code	Value	Unit	Source
chl	-7239.10 ± 1.50	kJ/mol	NIST Webbook
gf	66.19	kJ/mol	Joback Method
hf	-233.80 ± 1.70	kJ/mol	NIST Webbook
hfus	16.08	kJ/mol	Joback Method
hvap	52.90 ± 0.50	kJ/mol	NIST Webbook
hvap	53.90	kJ/mol	NIST Webbook
hvap	53.88	kJ/mol	NIST Webbook
hvap	54.10 ± 0.30	kJ/mol	NIST Webbook
hvap	54.10 ± 0.30	kJ/mol	NIST Webbook
hvap	55.00	kJ/mol	NIST Webbook
log10ws	-4.08		Crippen Method
logp	4.147		Crippen Method
mcvol	154.990	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinpol	1130.20		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1130.20		NIST Webbook
rinpol	1134.70		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1130.60		NIST Webbook

rinpol	1133.26		NIST Webbook
rinpol	1132.42		NIST Webbook
rinpol	1136.64		NIST Webbook
rinpol	1139.51		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1134.70		NIST Webbook
rinpol	1126.52		NIST Webbook
rinpol	1136.90		NIST Webbook
rinpol	1122.00		NIST Webbook
ripol	1309.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1288.00		NIST Webbook
ripol	1293.00		NIST Webbook
ripol	1299.00		NIST Webbook
ripol	1304.00		NIST Webbook
tb	472.15 ± 2.00	K	NIST Webbook
tb	469.40 ± 4.00	K	NIST Webbook
tb	474.80 ± 1.50	K	NIST Webbook
tb	477.00 ± 0.60	K	NIST Webbook
tc	665.19	K	Joback Method
tf	221.11	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.14	J/mol×K	665.19	Joback Method
cpg	366.87	J/mol×K	503.06	Joback Method
cpg	386.16	J/mol×K	535.48	Joback Method

cpg	404.50	J/mol×K	567.91	Joback Method
cpg	421.93	J/mol×K	600.34	Joback Method
cpg	438.46	J/mol×K	632.77	Joback Method
cpg	346.62	J/mol×K	470.63	Joback Method
dvisc	0.0085082	Pa×s	221.11	Joback Method
dvisc	0.0029690	Pa×s	262.70	Joback Method
dvisc	0.0013815	Pa×s	304.28	Joback Method
dvisc	0.0007727	Pa×s	345.87	Joback Method
dvisc	0.0004896	Pa×s	387.46	Joback Method
dvisc	0.0003389	Pa×s	429.04	Joback Method
dvisc	0.0002504	Pa×s	470.63	Joback Method
rho1	774.75	kg/m3	333.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rho1	782.14	kg/m3	323.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rho1	789.49	kg/m3	313.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rho1	796.82	kg/m3	303.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations

rhoI	800.48	kg/m3	298.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhoI	804.13	kg/m3	293.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhoI	807.78	kg/m3	288.15	Thermophysical Properties of Binary Mixtures of n-Dodecane with n-Alkylcyclohexanes: Experimental Measurements and Molecular Dynamics Simulations
rhoI	752.40	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
rhoI	759.90	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

rhoI	767.30	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
rhoI	774.74	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
rhoI	782.12	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
rhoI	789.47	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

rhoI	796.80	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
rhoI	804.11	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

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41752e+01
Coeff. B	-3.86144e+03
Coeff. C	-7.29520e+01
Temperature range (K), min.	351.00
Temperature range (K), max.	508.60

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C4292926&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 Alkylcyclohexane (n-Pentyl, n-Hexyl, n-Heptyl, n-Octyl, n-Nonyl, n-Decyl, and n-Dodecyl) with Cyclohexane: Experimental Measurements and Molecular Dynamics Simulations: <https://www.doi.org/10.1021/acs.jced.8b00692>
<https://www.doi.org/10.1021/acs.jced.8b01135>
https://en.wikipedia.org/wiki/Joback_method
<http://link.springer.com/article/10.1007/BF02311772>

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

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

rho: Liquid Density

rinpol: Non-polar retention indices

ripol: Polar retention indices

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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