

# Heptane, 2,2,4,6,6-pentamethyl-

Other names:	2,2,4,6,6-Pentamethylheptane Permethyl 99A
Inchi:	InChI=1S/C12H26/c1-10(8-11(2,3)4)9-12(5,6)7/h10H,8-9H2,1-7H3
InchiKey:	VKPSKYDESGTTFR-UHFFFAOYSA-N
Formula:	C12H26
SMILES:	CC(CC(C)(C)C)CC(C)(C)C
Mol. weight [g/mol]:	170.33
CAS:	13475-82-6

## Physical Properties

Property code	Value	Unit	Source
gf	53.40	kJ/mol	Joback Method
hf	-313.79	kJ/mol	Joback Method
hfus	8.48	kJ/mol	Joback Method
hvap	48.97	kJ/mol	NIST Webbook
hvap	49.00 ± 0.20	kJ/mol	NIST Webbook
log10ws	-4.12		Crippen Method
logp	4.495		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	985.00		NIST Webbook
rinpol	990.04		NIST Webbook
rinpol	992.84		NIST Webbook
rinpol	994.39		NIST Webbook
rinpol	987.85		NIST Webbook
rinpol	990.16		NIST Webbook
rinpol	992.02		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	985.00		NIST Webbook

rinpol	987.85		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	999.00		NIST Webbook
ripol	915.00		NIST Webbook
ripol	915.00		NIST Webbook
ripol	957.00		NIST Webbook
ripol	954.00		NIST Webbook
ripol	956.00		NIST Webbook
ripol	943.00		NIST Webbook
tb	467.06	K	Joback Method
tc	651.57	K	Joback Method
tf	206.18 ± 0.08	K	NIST Webbook
tf	206.23 ± 0.03	K	NIST Webbook
tf	206.23 ± 0.05	K	NIST Webbook
tf	206.18 ± 0.06	K	NIST Webbook
tf	203.20 ± 3.00	K	NIST Webbook
tf	206.23 ± 0.06	K	NIST Webbook
tf	206.17 ± 0.07	K	NIST Webbook
tf	206.18 ± 0.08	K	NIST Webbook
tf	203.00 ± 3.00	K	NIST Webbook
vc	0.679	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.05	J/molxK	467.06	Joback Method
cpg	431.10	J/molxK	497.81	Joback Method
cpg	450.08	J/molxK	528.56	Joback Method
cpg	468.04	J/molxK	559.31	Joback Method
cpg	485.02	J/molxK	590.07	Joback Method
cpg	501.08	J/molxK	620.82	Joback Method
cpg	516.26	J/molxK	651.57	Joback Method
cpl	350.98	J/molxK	298.15	NIST Webbook
cpl	350.98	J/molxK	298.15	NIST Webbook

dvisc	0.0003083	Paxs	425.02	Joback Method
dvisc	0.0005113	Paxs	382.99	Joback Method
dvisc	0.0009608	Paxs	340.95	Joback Method
dvisc	0.0021558	Paxs	298.91	Joback Method
dvisc	0.0063015	Paxs	256.88	Joback Method
dvisc	0.0002036	Paxs	467.06	Joback Method
dvisc	0.0280272	Paxs	214.84	Joback Method
rho1	730.90	kg/m3	313.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Direct Sugar to Hydrocarbon Diesel (DSH-76) and Binary Mixtures of N-Hexadecane and 2,2,4,6,6-Pentamethylheptane
rho1	723.50	kg/m3	323.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Direct Sugar to Hydrocarbon Diesel (DSH-76) and Binary Mixtures of N-Hexadecane and 2,2,4,6,6-Pentamethylheptane
rho1	716.10	kg/m3	333.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Direct Sugar to Hydrocarbon Diesel (DSH-76) and Binary Mixtures of N-Hexadecane and 2,2,4,6,6-Pentamethylheptane

rhoI	708.60	kg/m3	343.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Direct Sugar to Hydrocarbon Diesel (DSH-76) and Binary Mixtures of N-Hexadecane and 2,2,4,6,6-Pentamethylheptane
rhoI	700.90	kg/m3	353.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Direct Sugar to Hydrocarbon Diesel (DSH-76) and Binary Mixtures of N-Hexadecane and 2,2,4,6,6-Pentamethylheptane
rhoI	693.20	kg/m3	363.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Direct Sugar to Hydrocarbon Diesel (DSH-76) and Binary Mixtures of N-Hexadecane and 2,2,4,6,6-Pentamethylheptane
rhoI	685.50	kg/m3	373.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Direct Sugar to Hydrocarbon Diesel (DSH-76) and Binary Mixtures of N-Hexadecane and 2,2,4,6,6-Pentamethylheptane

rhoI	738.20	kg/m3	303.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Direct Sugar to Hydrocarbon Diesel (DSH-76) and Binary Mixtures of N-Hexadecane and 2,2,4,6,6-Pentamethylheptane
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rhoI	737.93	kg/m3	303.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of 2,2,4,6,6-Pentamethylheptane and 2,2,4,4,6,8,8-Heptamethylnonane at (293.15 to 373.15) K and 0.1 MPa and Comparisons with Alcohol-to-Jet Fuel
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rhoI	730.61	kg/m3	313.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of 2,2,4,6,6-Pentamethylheptane and 2,2,4,4,6,8,8-Heptamethylnonane at (293.15 to 373.15) K and 0.1 MPa and Comparisons with Alcohol-to-Jet Fuel
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rhoI	723.26	kg/m3	323.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of 2,2,4,6,6-Pentamethylheptane and 2,2,4,4,6,8,8-Heptamethylnonane at (293.15 to 373.15) K and 0.1 MPa and Comparisons with Alcohol-to-Jet Fuel
rhoI	715.86	kg/m3	333.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of 2,2,4,6,6-Pentamethylheptane and 2,2,4,4,6,8,8-Heptamethylnonane at (293.15 to 373.15) K and 0.1 MPa and Comparisons with Alcohol-to-Jet Fuel
rhoI	708.42	kg/m3	343.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of 2,2,4,6,6-Pentamethylheptane and 2,2,4,4,6,8,8-Heptamethylnonane at (293.15 to 373.15) K and 0.1 MPa and Comparisons with Alcohol-to-Jet Fuel

rhoI	700.70	kg/m3	353.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of 2,2,4,6,6-Pentamethylheptane and 2,2,4,4,6,8,8-Heptamethylnonane at (293.15 to 373.15) K and 0.1 MPa and Comparisons with Alcohol-to-Jet Fuel
rhoI	693.10	kg/m3	363.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of 2,2,4,6,6-Pentamethylheptane and 2,2,4,4,6,8,8-Heptamethylnonane at (293.15 to 373.15) K and 0.1 MPa and Comparisons with Alcohol-to-Jet Fuel
rhoI	715.80	kg/m3	333.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at 0.1 MPa

rhoI	775.80	kg/m3	253.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at 0.1 MPa
rhoI	748.80	kg/m3	288.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at 0.1 MPa
rhoI	745.20	kg/m3	293.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at 0.1 MPa
rhoI	737.90	kg/m3	303.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at 0.1 MPa



rhoI	730.60	kg/m3	313.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at 0.1 MPa
rhoI	745.50	kg/m3	293.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Direct Sugar to Hydrocarbon Diesel (DSH-76) and Binary Mixtures of N-Hexadecane and 2,2,4,6,6-Pentamethylheptane
rhoI	685.40	kg/m3	373.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of 2,2,4,6,6-Pentamethylheptane and 2,2,4,4,6,8,8-Heptamethylnonane at (293.15 to 373.15) K and 0.1 MPa and Comparisons with Alcohol-to-Jet Fuel
rhoI	723.20	kg/m3	323.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at 0.1 MPa

rhoI	745.21	kg/m3	293.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of 2,2,4,6,6-Pentamethylheptane and 2,2,4,4,6,8,8-Heptamethylnonane at (293.15 to 373.15) K and 0.1 MPa and Comparisons with Alcohol-to-Jet Fuel
speedsl	1089.30	m/s	323.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Dodecane with 2,2,4,6,6-Pentamethylheptane or 2,2,4,4,6,8,8-Heptamethylnonane
speedsl	1126.70	m/s	313.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Dodecane with 2,2,4,6,6-Pentamethylheptane or 2,2,4,4,6,8,8-Heptamethylnonane
speedsl	1164.80	m/s	303.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Dodecane with 2,2,4,6,6-Pentamethylheptane or 2,2,4,4,6,8,8-Heptamethylnonane

speedsl	1203.60	m/s	293.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Dodecane with 2,2,4,6,6-Pentamethylheptane or 2,2,4,4,6,8,8-Heptamethylnonane
speedsl	1052.50	m/s	333.15	Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Dodecane with 2,2,4,6,6-Pentamethylheptane or 2,2,4,4,6,8,8-Heptamethylnonane

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.33897e+01
Coeff. B	-3.15580e+03
Coeff. C	-9.13150e+01
Temperature range (K), min.	332.18
Temperature range (K), max.	481.97

## Sources

Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Dodecane with 2,2,4,6,6-Pentamethylheptane or 2,2,4,4,6,8,8-Heptamethylnonane: The Yaws Handbook of Vapor Pressure: Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at 0.1 MPa:

<https://www.doi.org/10.1021/je5000132>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

<https://www.doi.org/10.1021/je400839x>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C13475826&Units=SI>

<http://link.springer.com/article/10.1007/BF02311772>

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<https://www.doi.org/10.1021/acs.jced.8b00387>

<https://www.cheric.org/files/research/kdb/mol/mol172.mol>

Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Vapor Pressure of Binary Mixtures of 2,2,4,6,6-Pentamethylheptane and 2,2,4,4,6,8,8-Heptamethylnonane at (293.15 to 373.15) K and 0.1 MPa and Comparisons with Alcohol-to-Jet Fuel:

<https://www.doi.org/10.1021/je501141e>

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>cp<sub>l</sub>:</b>	Liquid phase heat capacity
<b>d<sub>visc</sub>:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10ws</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>p<sub>c</sub>:</b>	Critical Pressure
<b>p<sub>vap</sub>:</b>	Vapor pressure
<b>ρ<sub>l</sub>:</b>	Liquid Density
<b>ri<sub>npol</sub>:</b>	Non-polar retention indices
<b>ri<sub>pol</sub>:</b>	Polar retention indices
<b>speed<sub>s</sub>l:</b>	Speed of sound in fluid
<b>t<sub>b</sub>:</b>	Normal Boiling Point Temperature
<b>t<sub>c</sub>:</b>	Critical Temperature
<b>t<sub>f</sub>:</b>	Normal melting (fusion) point
<b>v<sub>c</sub>:</b>	Critical Volume

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