

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	49.00 ± 0.20	kJ/mol	NIST Webbook
hvap	48.97	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	997.00		NIST Webbook
rinpol	994.00		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	990.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	985.00		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	995.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	987.85		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	996.00		NIST Webbook
ripol	915.00		NIST Webbook
ripol	943.00		NIST Webbook
ripol	957.00		NIST Webbook
ripol	954.00		NIST Webbook
ripol	956.00		NIST Webbook
ripol	915.00		NIST Webbook
tb	467.06	K	Joback Method
tc	651.57	K	Joback Method
tf	206.18 ± 0.08	K	NIST Webbook
tf	203.20 ± 3.00	K	NIST Webbook
tf	206.17 ± 0.07	K	NIST Webbook
tf	203.00 ± 3.00	K	NIST Webbook
tf	206.18 ± 0.06	K	NIST Webbook
tf	206.23 ± 0.03	K	NIST Webbook
tf	206.18 ± 0.08	K	NIST Webbook
tf	206.23 ± 0.05	K	NIST Webbook
tf	206.23 ± 0.06	K	NIST Webbook
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0021558	Paxs	298.91	Joback Method	
dvisc	0.0009608	Paxs	340.95	Joback Method	
dvisc	0.0005113	Paxs	382.99	Joback Method	
dvisc	0.0003083	Paxs	425.02	Joback Method	
dvisc	0.0002036	Paxs	467.06	Joback Method	
dvisc	0.0280272	Paxs	214.84	Joback Method	
dvisc	0.0063015	Paxs	256.88	Joback Method	
rho1	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	
rho1	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	
rho1	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
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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
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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
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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	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	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	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	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	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	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
rhoI	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
rhoI	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
rhoI	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	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
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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	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
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
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

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

NIST Webbook:
McGowan Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C13475826&Units=SI>
<http://link.springer.com/article/10.1007/BF02311772>
<https://www.doi.org/10.1021/je5000132>
https://www.chemeo.com/doc/models/crippen_log10ws
<https://www.doi.org/10.1021/je400839x>
<https://www.doi.org/10.1021/acs.jced.8b00387>
<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<https://www.cheric.org/files/research/kdb/mol/mol172.mol>

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 (1) in 2,2,4,6,6-Pentamethylheptane (2) or 2,2,4,4,6,8,8-Heptamethylnonane (2) at 0.1 MPa:

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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
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
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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