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	996.00		NIST Webbook
rinpol	985.00		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	997.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	990.00		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	995.00		NIST Webbook
rinpol	987.85		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	992.02		NIST Webbook
rinpol	997.00		NIST Webbook
ripol	957.00		NIST Webbook
ripol	915.00		NIST Webbook
ripol	915.00		NIST Webbook
ripol	956.00		NIST Webbook
ripol	954.00		NIST Webbook
ripol	943.00		NIST Webbook
tb	467.06	K	Joback Method
tc	651.57	K	Joback Method
tf	203.20 ± 3.00	K	NIST Webbook
tf	203.00 ± 3.00	K	NIST Webbook
tf	206.23 ± 0.05	K	NIST Webbook
tf	206.17 ± 0.07	K	NIST Webbook
tf	206.23 ± 0.03	K	NIST Webbook
tf	206.18 ± 0.06	K	NIST Webbook
tf	206.18 ± 0.08	K	NIST Webbook
tf	206.18 ± 0.08	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/mol×K	590.07	Joback Method
cpg	501.08	J/mol×K	620.82	Joback Method
cpg	468.04	J/mol×K	559.31	Joback Method
cpg	516.26	J/mol×K	651.57	Joback Method
cpg	411.05	J/mol×K	467.06	Joback Method
cpg	431.10	J/mol×K	497.81	Joback Method
cpg	450.08	J/mol×K	528.56	Joback Method
cpl	350.98	J/mol×K	298.15	NIST Webbook
cpl	350.98	J/mol×K	298.15	NIST Webbook

dvisc	0.0021558	Pa×s	298.91	Joback Method
dvisc	0.0009608	Pa×s	340.95	Joback Method
dvisc	0.0005113	Pa×s	382.99	Joback Method
dvisc	0.0003083	Pa×s	425.02	Joback Method
dvisc	0.0002036	Pa×s	467.06	Joback Method
dvisc	0.0280272	Pa×s	214.84	Joback Method
dvisc	0.0063015	Pa×s	256.88	Joback Method
rhol	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
rhol	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
rhol	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

rhol	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
rhol	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
rhol	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

rhol	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
rhol	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
rhol	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

rhol	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
rhol	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
rhol	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
rhol	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

rhol	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
rhol	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
rhol	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
rhol	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

rhol	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
rhol	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
rhol	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
rhol	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

rhol	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
rhol	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
rhol	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

rhol	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(Pvp) = 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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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:	https://www.doi.org/10.1021/je400839x
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13475826&Units=SI
Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n-Hexylbenzene (1) or n-Butylbenzene (1) with 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/acs.jced.8b00387
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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:	https://www.doi.org/10.1021/je5000132

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	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 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

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
rhol:	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