Heptane, 2-methyl-

Other names: (CH3)2CH(CH2)4CH3
2-METHYLHEPTANE
METHYLHEPTANE
Inchi: InChI=1S/C8H18/c1-4-5-6-7-8(2)3/h8H,4-7H2,1-3H3
InchiKey: JVSWJIKNEAIKJW-UHFFFAOYSA-N
Formula: C8H18
SMILES: CCCCCC(C)C
Mol. weight [g/mol]: 114.23
CAS: 592-27-8

Physical Properties

Property code	Value	Unit	Source
af	0.3780		KDB
ap	347.150	K	KDB
chl	-5274.60	kJ/mol	NIST Webbook
chl	-5465.50 ± 1.20	kJ/mol	NIST Webbook
chl	-5447.10	kJ/mol	NIST Webbook
gf	12.77	kJ/mol	KDB
hcg	5465.48	kJ/mol	KDB
hcn	5069.335	kJ/mol	KDB
hf	-215.60	kJ/mol	KDB
hf	-215.50 ± 1.30	kJ/mol	NIST Webbook
hfl	-255.20 ± 1.30	kJ/mol	NIST Webbook
hfus	12.95	kJ/mol	Joback Method
hvap	39.67	kJ/mol	NIST Webbook
hvap	39.70	kJ/mol	NIST Webbook
hvap	39.80 ± 0.10	kJ/mol	NIST Webbook
hvap	33.00	kJ/mol	NIST Webbook
hvap	39.72	kJ/mol	NIST Webbook
hvap	39.70 ± 0.10	kJ/mol	NIST Webbook
ie	9.76	eV	NIST Webbook
ie	9.74 ± 0.15	eV	NIST Webbook
ie	9.84 ± 0.10	eV	NIST Webbook
ie	9.84 ± 0.10	eV	NIST Webbook
log10ws	-5.08		Estimated Solubility Method
log10ws	-5.08		Aqueous Solubility Prediction Method

logp	3.223		Crippen Method
mcvol	123.580	ml/mol	McGowan Method
pc	2500.00	kPa	KDB
pc	2484.20 ± 40.53	kPa	NIST Webbook
pc	2500.00 ± 40.00	kPa	NIST Webbook
pc	2500.00 ± 20.00	kPa	NIST Webbook
rhoc	234.17 ± 4.57	kg/m3	NIST Webbook
rhoc	234.17 ± 2.28	kg/m3	NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	762.00		NIST Webbook
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rinpol	758.54		NIST Webbook
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rinpol	768.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	764.30		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	765.00		NIST Webbook

rinpol	766.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	776.21	NIST Webbook
rinpol	760.00	NIST Webbook
rinpol	761.00	NIST Webbook
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rinpol	766.21	NIST Webbook
rinpol	765.99	NIST Webbook
rinpol	767.12	NIST Webbook
rinpol	766.99	NIST Webbook
rinpol	766.78	NIST Webbook
rinpol	765.50	NIST Webbook
rinpol	765.50	NIST Webbook
rinpol	765.90	NIST Webbook
rinpol	763.00	NIST Webbook
rinpol	763.50	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	763.03	NIST Webbook
rinpol	763.00	NIST Webbook
rinpol	762.36	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	760.00	NIST Webbook
rinpol	762.25	NIST Webbook
rinpol	761.10	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	764.10	NIST Webbook
rinpol	762.50	NIST Webbook
rinpol	761.79	NIST Webbook
rinpol	761.38	NIST Webbook
rinpol	766.90	NIST Webbook
rinpol	766.50	NIST Webbook
rinpol	778.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	769.00	NIST Webbook
rinpol	764.10	NIST Webbook
rinpol	760.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	764.10	NIST Webbook
rinpol	759.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	765.50	NIST Webbook
rinpol	765.80	NIST Webbook
rinpol	765.00	NIST Webbook

rinpol	766.00	NIST Webbook
rinpol	766.30	NIST Webbook
rinpol	765.00	NIST Webbook
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rinpol	765.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	764.70	NIST Webbook
rinpol	765.60	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	766.20	NIST Webbook
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rinpol	765.00	NIST Webbook
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rinpol	765.00	NIST Webbook
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rinpol	764.00	NIST Webbook
rinpol	766.40	NIST Webbook
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rinpol	766.00	NIST Webbook
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rinpol	764.90	NIST Webbook
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rinpol	764.60	NIST Webbook
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rinpol	765.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	772.52	NIST Webbook
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rinpol	765.00		NIST Webbook
rinpol	765.10		NIST Webbook
rinpol	764.00		NIST Webbook
rinpol	761.00		NIST Webbook
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rinpol	765.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	767.00		NIST Webbook
ripol	750.00		NIST Webbook
ripol	764.00		NIST Webbook
ripol	764.00		NIST Webbook
sg	459.49 ± 0.88	J/mol×K	NIST Webbook
sl	356.39	J/mol×K	NIST Webbook
tb	390.80 ± 0.20	K	NIST Webbook
tb	390.81	K	KDB
tb	390.80	K	NIST Webbook
tb	390.80	K	NIST Webbook
tb	390.90 ± 1.00	K	NIST Webbook
tb	390.78 ± 0.20	K	NIST Webbook
tb	391.00 ± 3.00	K	NIST Webbook
tb	390.00 ± 3.00	K	NIST Webbook
tb	390.85 ± 0.20	K	NIST Webbook
tb	390.40 ± 0.30	K	NIST Webbook
tb	390.79 ± 0.10	K	NIST Webbook

tb	390.90 ± 0.20	K	NIST Webbook
tb	391.15 ± 1.00	K	NIST Webbook
tb	391.00 ± 2.00	K	NIST Webbook
tb	389.15 ± 0.30	K	NIST Webbook
tb	390.65 ± 1.50	K	NIST Webbook
tb	391.00 ± 1.00	K	NIST Webbook
tb	390.35 ± 0.50	K	NIST Webbook
tb	390.35 ± 0.60	K	NIST Webbook
tb	391.00 ± 0.30	K	NIST Webbook
tb	389.85 ± 0.50	K	NIST Webbook
tb	391.25 ± 0.30	K	NIST Webbook
tb	391.15 ± 0.30	K	NIST Webbook
tb	390.79 ± 0.10	K	NIST Webbook
tb	390.80 ± 0.30	K	NIST Webbook
tb	390.85 ± 0.10	K	NIST Webbook
tb	390.00 ± 3.00	K	NIST Webbook
tb	390.15 ± 1.50	K	NIST Webbook
tb	390.15 ± 1.00	K	NIST Webbook
tb	390.75 ± 0.50	K	NIST Webbook
tb	390.85 ± 0.20	K	NIST Webbook
tb	390.55 ± 0.50	K	NIST Webbook
tb	390.79 ± 0.01	K	NIST Webbook
tb	390.90 ± 0.20	K	NIST Webbook
tb	390.90 ± 0.15	K	NIST Webbook
tb	390.86 ± 0.20	K	NIST Webbook
tb	389.75 ± 0.60	K	NIST Webbook
tb	390.85 ± 0.30	K	NIST Webbook
tb	391.60 ± 2.00	K	NIST Webbook
tc	559.57 ± 0.20	K	NIST Webbook
tc	559.56 ± 0.40	K	NIST Webbook
tc	559.70 ± 0.20	K	NIST Webbook
tc	559.70 ± 0.10	K	NIST Webbook
tc	559.60	K	NIST Webbook
tc	559.70	K	KDB
tf	163.32 ± 0.15	K	NIST Webbook
tf	164.16	K	KDB
tf	165.52	K	Aqueous Solubility Prediction Method
tf	163.59 ± 0.20	K	NIST Webbook
tf	163.59 ± 0.30	K	NIST Webbook
tf	163.52 ± 0.20	K	NIST Webbook
tf	163.52 ± 0.30	K	NIST Webbook
tf	163.90 ± 0.02	K	NIST Webbook
tf	164.03 ± 0.06	K	NIST Webbook
tf	164.11 ± 0.05	K	NIST Webbook

tf	164.02 ± 0.09	K	NIST Webbook
tf	161.85 ± 1.50	K	NIST Webbook
tf	162.15 ± 2.00	K	NIST Webbook
tf	160.00 ± 0.30	K	NIST Webbook
tf	163.65 ± 0.10	K	NIST Webbook
tf	163.55 ± 0.50	K	NIST Webbook
tt	164.14 ± 0.02	K	NIST Webbook
tt	154.91 ± 0.03	K	NIST Webbook
tt	154.87 ± 0.04	K	NIST Webbook
tt	154.87 ± 0.05	K	NIST Webbook
tt	154.91 ± 0.02	K	NIST Webbook
tt	164.14 ± 0.40	K	NIST Webbook
tt	164.14 ± 0.02	K	NIST Webbook
tt	163.15 ± 0.02	K	NIST Webbook
tt	164.19 ± 0.01	K	NIST Webbook
tt	164.18 ± 0.04	K	NIST Webbook
vc	0.488	m3/kmol	NIST Webbook
vc	0.488	m3/kmol	KDB
zc	0.2621610		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.52	J/mol×K	448.15	NIST Webbook
cpg	230.06	J/mol×K	373.15	NIST Webbook
cpg	248.37	J/mol×K	408.15	NIST Webbook
cpg	186.13	J/mol×K	298.15	NIST Webbook
cpg	202.07	J/mol×K	323.15	NIST Webbook
cpl	252.00	J/mol×K	298.15	NIST Webbook
cpl	251.58	J/mol×K	298.15	NIST Webbook
dvisc	0.0007454	Pa×s	273.46	Joback Method
dvisc	0.0013776	Pa×s	237.28	Joback Method
dvisc	0.0002373	Pa×s	382.00	Joback Method
dvisc	0.0105616	Pa×s	164.92	Joback Method
dvisc	0.0003209	Pa×s	345.82	Joback Method
dvisc	0.0004656	Pa×s	309.64	Joback Method
dvisc	0.0031758	Pa×s	201.10	Joback Method
hfust	11.92	kJ/mol	64.19	NIST Webbook
hfust	11.92	kJ/mol	164.20	NIST Webbook
hfust	11.92	kJ/mol	164.20	NIST Webbook
hvapt	33.26	kJ/mol	390.80	NIST Webbook

hvapt	33.81	kJ/mol	390.80	KDB
hvapt	41.60	kJ/mol	258.00	NIST Webbook
hvapt	38.70 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	37.30 ± 0.10	kJ/mol	333.00	NIST Webbook
hvapt	36.00 ± 0.10	kJ/mol	353.00	NIST Webbook
hvapt	38.10	kJ/mol	353.00	NIST Webbook
hvapt	39.80	kJ/mol	338.50	NIST Webbook
rfi	1.39257		298.15	KDB
rhol	702.00	kg/m3	289.00	KDB
sfust	72.60	J/mol×K	64.19	NIST Webbook
srf	0.02	N/m	298.20	KDB
tcondl	0.12	W/m×K	277.77	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.11	W/m×K	313.83	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.11	W/m×K	296.16	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.11	W/m×K	295.95	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.11	W/m×K	295.72	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.12	W/m×K	277.96	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)

tcondl	0.11	W/m×K	328.23	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.11	W/m×K	314.07	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.12	W/m×K	277.53	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.11	W/m×K	314.30	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.11	W/m×K	327.74	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.12	W/m×K	259.51	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.12	W/m×K	259.12	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)

tcondl	0.11	W/m×K	328.00	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.12	W/m×K	259.33	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
volm	1.64e-04	m3/mol	298.15	Thermodynamic study of (perfluoroalkane + alkane) mixtures: Excess and solvation enthalpies
volm	1.63e-04	m3/mol	288.05	Thermodynamic study of (perfluoroalkane + alkane) mixtures: Excess and solvation enthalpies

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	389.20	K	101.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43957e+01
Coeff. B	-3.39364e+03
Coeff. C	-4.37100e+01
Temperature range (K), min.	284.25
Temperature range (K), max.	417.28

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.36210e+01
Coeff. B	-7.47230e+03
Coeff. C	-1.02064e+01
Coeff. D	6.78071e-06
Temperature range (K), min.	164.16
Temperature range (K), max.	559.64

Datasets

Molar heat capacity at constant pressure, J/K/mol

Temperature, K - Liquid	Pressure, kPa - Liquid	Molar heat capacity at constant pressure, J/K/mol - Liquid
293.15	100.00	236.20
293.15	5000.00	233.80
293.15	10000.00	231.70
293.15	15000.00	229.10
293.15	20000.00	228.00
293.15	25000.00	224.80
313.15	100.00	249.60
313.15	5000.00	246.80
313.15	10000.00	245.10
313.15	15000.00	243.20
313.15	20000.00	240.80
313.15	25000.00	235.10

Reference *https://www.doi.org/10.1016/j.jct.2011.08.012*

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid

298.15	100.00	693.9
Reference		*https://www.doi.org/10.1016/j.jct.2017.07.026*

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C592278&Units=SI
Thermodynamic characterization of the mixture (1-butanol + iso-octane):	https://www.doi.org/10.1016/j.jct.2011.08.012
Densities, viscosities, and isobaric heat capacities at high pressures:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Liquid liquid equilibria of imidazolium based ionic liquid + pyridine + hydrocarbon at 298.15 K: Experiments and correlations:	https://www.doi.org/10.1016/j.fluid.2012.03.023
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8):	https://www.doi.org/10.1021/je020125e
Estimated Solubility Methods:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Thermodynamic study of (perfluoroalkane + alkane) mixtures: Excess and solvation enthalpies:	https://www.doi.org/10.1016/j.jct.2007.04.002
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=47
Conformational analysis of branched alkanes using limiting partial molar volumes:	https://www.doi.org/10.1016/j.jct.2017.07.026
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=47

Legend

af:	Acentric Factor
ap:	Aniline Point
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
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
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
hvapt:	Enthalpy of vaporization at a given temperature

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
volm:	Molar Volume
zc:	Critical Compressibility