Hexane, 2-methyl-

Other names:	2-Methylhexane
	ISOHEPTANE
Inchi:	InChI=1S/C7H16/c1-4-5-6-7(2)3/h7H,4-6H2,1-3H3
InchiKey:	GXDHCNNESPLIKD-UHFFFAOYSA-N
Formula:	C7H16
SMILES:	CCCCC(C)C
Mol. weight [g/mol]:	100.20
CAS:	591-76-4

Physical Properties

Property code	Value	Unit	Source
af	0.3290		KDB
ap	347.150	K	KDB
chl	-4811.50 ± 1.20	kJ/mol	NIST Webbook
chl	-4810.00 ± 1.00	kJ/mol	NIST Webbook
dm	0.00	debye	KDB
gf	3.22	kJ/mol	KDB
hcg	4811.48	kJ/mol	KDB
hcn	4459.350	kJ/mol	KDB
hf	-195.00 ± 1.30	kJ/mol	NIST Webbook
hf	-196.20	kJ/mol	NIST Webbook
hf	-195.10	kJ/mol	KDB
hfl	-229.80 ± 1.30	kJ/mol	NIST Webbook
hfl	-231.00 ± 1.00	kJ/mol	NIST Webbook
hfus	10.36	kJ/mol	Joback Method
hvap	34.80	kJ/mol	NIST Webbook
hvap	34.80	kJ/mol	NIST Webbook
hvap	34.90 ± 0.10	kJ/mol	NIST Webbook
hvap	34.98	kJ/mol	NIST Webbook
log10ws	-2.51		Crippen Method
logp	2.833		Crippen Method
mcvol	109.490	ml/mol	McGowan Method
pc	2740.00 ± 20.00	kPa	NIST Webbook
pc	2740.00	kPa	KDB
pc	2750.00 ± 25.00	kPa	NIST Webbook
pc	2732.80 ± 40.53	kPa	NIST Webbook
pc	2756.04 ± 50.66	kPa	NIST Webbook

rhoc	238.48 ± 2.00	kg/m3	NIST Webbook
rhoc	238.48 ± 5.01	kg/m3	NIST Webbook
rinpol	667.00		NIST Webbook
rinpol	666.40		NIST Webbook
rinpol	667.10		NIST Webbook
rinpol	666.10		NIST Webbook
rinpol	667.50		NIST Webbook
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ripol	650.00		NIST Webbook
ripol	650.00		NIST Webbook
sg	419.99	J/mol×K	NIST Webbook
sl	315.10	J/mol×K	NIST Webbook
sl	323.34	J/mol×K	NIST Webbook
sl	314.60	J/mol×K	NIST Webbook
tb	363.19	K	KDB
tc	530.40	K	KDB
tf	154.85 ± 0.02	K	NIST Webbook
tf	154.25 ± 0.20	K	NIST Webbook
tf	154.91 ± 0.30	K	NIST Webbook
tf	154.05 ± 0.50	K	NIST Webbook
tf	154.05 ± 0.50	K	NIST Webbook
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tf	154.89 ± 0.20	K	NIST Webbook
tf	154.90	K	KDB
tf	154.87 ± 0.02	K	NIST Webbook
tf	154.86 ± 0.04	K	NIST Webbook
tf	154.88 ± 0.02	K	NIST Webbook
tf	154.86 ± 0.03	K	NIST Webbook
tt	154.90 ± 0.02	K	NIST Webbook
tt	154.86 ± 0.04	K	NIST Webbook
tt	154.90 ± 0.06	K	NIST Webbook
tt	154.86 ± 0.09	K	NIST Webbook

tt	154.00 ± 0.20	K	NIST Webbook
tt	154.00 ± 0.20	K	NIST Webbook
vc	0.421	m3/kmol	NIST Webbook
vc	0.421	m3/kmol	KDB
zc	0.2615730		KDB
zra	0.26		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.02	J/mol×K	359.12	Joback Method
cpg	260.72	J/mol×K	526.54	Joback Method
cpg	240.13	J/mol×K	470.73	Joback Method
cpg	229.23	J/mol×K	442.83	Joback Method
cpg	217.92	J/mol×K	414.93	Joback Method
cpg	206.19	J/mol×K	387.02	Joback Method
cpg	250.62	J/mol×K	498.63	Joback Method
cpl	219.20	J/mol×K	292.40	NIST Webbook
cpl	222.92	J/mol×K	298.15	NIST Webbook
dvisc	0.0004548	Pa×s	290.63	Joback Method
dvisc	0.0007226	Pa×s	256.38	Joback Method
dvisc	0.0013243	Pa×s	222.14	Joback Method
dvisc	0.0099972	Pa×s	153.65	Joback Method
dvisc	0.0030264	Pa×s	187.90	Joback Method
dvisc	0.0003156	Pa×s	324.88	Joback Method
dvisc	0.0002348	Pa×s	359.12	Joback Method
hfust	8.87	kJ/mol	154.00	NIST Webbook
hfust	8.87	kJ/mol	154.00	NIST Webbook
hfust	9.18	kJ/mol	154.90	NIST Webbook
hfust	9.18	kJ/mol	154.90	NIST Webbook
hfust	9.18	kJ/mol	154.90	NIST Webbook
hvapt	30.67	kJ/mol	363.20	KDB
hvapt	32.70 ± 0.10	kJ/mol	333.00	NIST Webbook
hvapt	33.90 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	34.80	kJ/mol	327.50	NIST Webbook
hvapt	34.60	kJ/mol	330.50	NIST Webbook
hvapt	30.62	kJ/mol	363.20	NIST Webbook
hvapt	31.30 ± 0.10	kJ/mol	353.00	NIST Webbook
rfi	1.38227		298.15	KDB
rhol	679.00	kg/m3	293.00	KDB
sfust	57.60	J/mol×K	154.00	NIST Webbook

sfust	57.60	J/mol×K	154.00	NIST Webbook	
sfust	59.29	J/mol×K	154.90	NIST Webbook	
srf	0.02	N/m	298.20	KDB	
tcondl	0.10	W/m×K	337.10	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.11	W/m×K	296.46	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.11	W/m×K	296.93	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.12	W/m×K	276.39	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.10	W/m×K	317.40	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.12	W/m×K	276.00	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.12	W/m×K	275.56	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	

tcondl	0.12	W/m×K	257.02	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.12	W/m×K	256.67	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.12	W/m×K	256.24	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.10	W/m×K	317.92	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.10	W/m×K	318.35	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.10	W/m×K	338.11	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.10	W/m×K	337.65	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	

tcondl	0.11	W/m×K	297.40	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42374e+01
Coeff. B	-3.08596e+03
Coeff. C	-4.23820e+01
Temperature range (K), min.	263.60
Temperature range (K), max.	388.11

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.26032e+01
Coeff. B	-7.22527e+03
Coeff. C	-1.17722e+01
Coeff. D	9.94213e-06
Temperature range (K), min.	154.90
Temperature range (K), max.	530.37

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8):	https://www.doi.org/10.1021/je020125e
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=39
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C591764&Units=SI
KDB:	https://www.cheric.org/files/research/kdb/mol/mol39.mol

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
ap:	Aniline Point
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
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
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
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

zc:	Critical Compressibility
zra:	Rackett Parameter

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