Heptane, 3-methyl-

Other names: (3RS)-3-methylheptane
2-ETHYLHEXANE
3-METHYLHEPTANE
Inchi: InChI=1S/C8H18/c1-4-6-7-8(3)5-2/h8H,4-7H2,1-3H3
InchiKey: LAIUFBWHERIJIH-UHFFFAOYSA-N
Formula: C8H18
SMILES: CCCCC(C)CC
Mol. weight [g/mol]: 114.23
CAS: 589-81-1

Physical Properties

Property code	Value	Unit	Source
af	0.3700		KDB
ap	345.350	K	KDB
chl	-5468.20 ± 1.30	kJ/mol	NIST Webbook
gf	13.73	kJ/mol	KDB
hcg	5468.15	kJ/mol	KDB
hcn	5072.012	kJ/mol	KDB
hf	-212.80	kJ/mol	KDB
hf	-212.60 ± 1.10	kJ/mol	NIST Webbook
hfl	-252.50 ± 1.10	kJ/mol	NIST Webbook
hfus	12.95	kJ/mol	Joback Method
hvap	39.83	kJ/mol	NIST Webbook
hvap	39.80 ± 0.20	kJ/mol	NIST Webbook
hvap	39.88	kJ/mol	NIST Webbook
hvap	39.80 ± 0.10	kJ/mol	NIST Webbook
hvap	39.80	kJ/mol	NIST Webbook
log10ws	-5.16		Estimated Solubility Method
log10ws	-5.16		Aqueous Solubility Prediction Method
logp	3.223		Crippen Method
mcvol	123.580	ml/mol	McGowan Method
pc	2550.00 ± 40.00	kPa	NIST Webbook
pc	2550.00	kPa	KDB
pc	2546.00 ± 40.53	kPa	NIST Webbook
rhoc	245.59 ± 4.57	kg/m3	NIST Webbook
rhoc	245.59 ± 4.57	kg/m3	NIST Webbook

rinpol	773.30	NIST Webbook
rinpol	770.31	NIST Webbook
rinpol	764.58	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	773.79	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	773.80	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	763.50	NIST Webbook
rinpol	771.90	NIST Webbook
rinpol	776.60	NIST Webbook
rinpol	778.00	NIST Webbook
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rinpol	774.00	NIST Webbook
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rinpol	772.00	NIST Webbook
rinpol	772.80	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	773.50	NIST Webbook
rinpol	773.90	NIST Webbook
rinpol	774.10	NIST Webbook
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rinpol	772.00	NIST Webbook
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rinpol	773.00	NIST Webbook
rinpol	762.00	NIST Webbook
rinpol	772.00	NIST Webbook

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rinpol	773.00	NIST Webbook
rinpol	772.80	NIST Webbook
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rinpol	773.00	NIST Webbook
rinpol	775.11	NIST Webbook
rinpol	775.75	NIST Webbook
rinpol	776.18	NIST Webbook
rinpol	774.38	NIST Webbook
rinpol	774.76	NIST Webbook
rinpol	773.00	NIST Webbook
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rinpol	771.70	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	774.30	NIST Webbook
rinpol	769.27	NIST Webbook
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rinpol	769.00	NIST Webbook
rinpol	770.31	NIST Webbook
rinpol	771.67	NIST Webbook
rinpol	770.68	NIST Webbook
rinpol	770.98	NIST Webbook
rinpol	771.00	NIST Webbook
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rinpol	773.70	NIST Webbook
rinpol	773.30	NIST Webbook
rinpol	772.90	NIST Webbook
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rinpol	773.02	NIST Webbook
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rinpol	766.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	769.00		NIST Webbook
rinpol	775.00		NIST Webbook
ripol	764.00		NIST Webbook
ripol	764.00		NIST Webbook
sg	465.89 ± 0.84	J/mol×K	NIST Webbook
sl	362.60	J/mol×K	NIST Webbook
tb	392.09	K	KDB
tc	563.60	K	KDB
tc	563.70	K	NIST Webbook
tc	563.60 ± 0.50	K	NIST Webbook
tc	563.60 ± 0.40	K	NIST Webbook
tf	152.60	K	KDB
tt	152.65 ± 0.01	K	NIST Webbook
vc	0.464	m3/kmol	NIST Webbook
vc	0.464	m3/kmol	KDB

zc	0.2524940	KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.38	J/mol×K	521.33	Joback Method
cpg	258.44	J/mol×K	437.73	Joback Method
cpg	270.88	J/mol×K	465.60	Joback Method
cpg	282.86	J/mol×K	493.46	Joback Method
cpg	305.46	J/mol×K	549.20	Joback Method
cpg	232.14	J/mol×K	382.00	Joback Method
cpg	245.53	J/mol×K	409.87	Joback Method
cpl	249.66	J/mol×K	298.15	NIST Webbook
cpl	250.20	J/mol×K	298.15	NIST Webbook
dvisc	0.0105616	Pa×s	164.92	Joback Method
dvisc	0.0013776	Pa×s	237.28	Joback Method
dvisc	0.0004656	Pa×s	309.64	Joback Method
dvisc	0.0003209	Pa×s	345.82	Joback Method
dvisc	0.0002373	Pa×s	382.00	Joback Method
dvisc	0.0007454	Pa×s	273.46	Joback Method
dvisc	0.0031758	Pa×s	201.10	Joback Method
hfust	11.70	kJ/mol	152.60	NIST Webbook
hfust	11.67	kJ/mol	152.60	NIST Webbook
hvapt	41.60	kJ/mol	262.00	NIST Webbook
hvapt	33.89	kJ/mol	392.10	KDB
hvapt	33.66	kJ/mol	392.10	NIST Webbook
hvapt	40.10	kJ/mol	339.50	NIST Webbook
hvapt	38.30	kJ/mol	354.50	NIST Webbook
rfi	1.39610		298.15	KDB
rhol	706.00	kg/m3	293.00	KDB
srf	0.02	N/m	298.20	KDB
tcondl	0.12	W/m×K	277.99	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)

tcondl	0.11	W/m×K	331.93	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.11	W/m×K	332.21	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.11	W/m×K	332.51	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.11	W/m×K	316.12	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.13	W/m×K	259.32	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.13	W/m×K	259.08	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.11	W/m×K	315.84	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	

tcondl	0.11	W/m×K	315.56	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.11	W/m×K	297.91	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.12	W/m×K	297.63	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.12	W/m×K	297.36	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.13	W/m×K	259.58	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.12	W/m×K	278.23	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.12	W/m×K	278.37	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	1.43862e+01
Coeff. B	-3.40203e+03
Coeff. C	-4.37910e+01
Temperature range (K), min.	285.09
Temperature range (K), max.	418.68

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.08909e+01
Coeff. B	-7.77747e+03
Coeff. C	-1.13291e+01
Coeff. D	7.90061e-06
Temperature range (K), min.	152.60
Temperature range (K), max.	563.67

Sources

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=48

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=48

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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 Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C589811&Units=SI

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
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
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

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