Heptane, 4-methyl-

Other names:	(n-C3H7)2CHCH3
	4-Methylheptane
Inchi:	InChI=1S/C8H18/c1-4-6-8(3)7-5-2/h8H,4-7H2,1-3H3
InchiKey:	CHBAWFGIXDBEBT-UHFFFAOYSA-N
Formula:	C8H18
SMILES:	CCCC(C)CCC
Mol. weight [g/mol]:	114.23
CAS:	589-53-7

Physical Properties

Property code	Value	Unit	Source
af	0.3710		KDB
ap	344.750	K	KDB
chl	-5468.90 ± 1.00	kJ/mol	NIST Webbook
gf	16.75	kJ/mol	KDB
hcg	5468.86	kJ/mol	KDB
hcn	5072.724	kJ/mol	KDB
hf	-212.20	kJ/mol	KDB
hf	-212.10 ± 1.20	kJ/mol	NIST Webbook
hfl	-251.80 ± 1.20	kJ/mol	NIST Webbook
hfus	12.95	kJ/mol	Joback Method
hvap	39.67	kJ/mol	NIST Webbook
hvap	39.70 ± 0.10	kJ/mol	NIST Webbook
hvap	39.70	kJ/mol	NIST Webbook
hvap	39.70 ± 0.10	kJ/mol	NIST Webbook
hvap	39.75	kJ/mol	NIST Webbook
hvap	33.80 ± 0.08	kJ/mol	NIST Webbook
log10ws	-2.93		Crippen Method
logp	3.223		Crippen Method
mcvol	123.580	ml/mol	McGowan Method
pc	2541.90 ± 40.53	kPa	NIST Webbook
pc	2540.00 ± 40.00	kPa	NIST Webbook
pc	2540.00	kPa	KDB
rhoc	239.88 ± 4.57	kg/m3	NIST Webbook
rhoc	239.88 ± 4.57	kg/m3	NIST Webbook
rinpol	762.50		NIST Webbook
rinpol	768.00		NIST Webbook

rinpol	768.00	NIST Webbook
rinpol	767.00	NIST Webbook
rinpol	757.00	NIST Webbook
rinpol	768.00	NIST Webbook
rinpol	767.00	NIST Webbook
rinpol	767.20	NIST Webbook
rinpol	768.10	NIST Webbook
rinpol	767.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	767.00	NIST Webbook
rinpol	768.00	NIST Webbook
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rinpol	767.70	NIST Webbook
rinpol	766.80	NIST Webbook
rinpol	768.50	NIST Webbook
rinpol	767.75	NIST Webbook
rinpol	768.05	NIST Webbook
rinpol	768.28	NIST Webbook
rinpol	767.16	NIST Webbook
rinpol	767.53	NIST Webbook
rinpol	767.77	NIST Webbook
rinpol	762.00	NIST Webbook
rinpol	777.73	NIST Webbook
rinpol	756.00	NIST Webbook
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rinpol	767.00	NIST Webbook
rinpol	768.00	NIST Webbook
rinpol	768.10	NIST Webbook
rinpol	768.00	NIST Webbook
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rinpol	767.20		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	766.80		NIST Webbook
rinpol	768.00		NIST Webbook
ripol	790.00		NIST Webbook
ripol	764.00		NIST Webbook
ripol	768.00		NIST Webbook
tb	390.76 ± 0.30	K	NIST Webbook
tb	391.15 ± 2.00	K	NIST Webbook
tb	391.15 ± 0.60	K	NIST Webbook
tb	390.87	K	KDB
tb	391.15 ± 1.00	K	NIST Webbook
tb	391.15 ± 0.20	K	NIST Webbook
tb	391.15 ± 0.40	K	NIST Webbook
tb	390.90	K	NIST Webbook
tb	390.90	K	NIST Webbook
tb	390.70 ± 2.00	K	NIST Webbook
tb	390.86 ± 0.20	K	NIST Webbook
tb	390.80 ± 0.20	K	NIST Webbook
tb	390.78 ± 0.20	K	NIST Webbook
tb	390.65 ± 0.50	K	NIST Webbook
tb	390.86 ± 0.20	K	NIST Webbook
tb	390.78 ± 0.15	K	NIST Webbook
tb	390.65 ± 0.30	K	NIST Webbook
tb	390.65 ± 0.30	K	NIST Webbook
tb	390.65 ± 0.60	K	NIST Webbook
tb	390.85 ± 0.01	K	NIST Webbook
tb	391.15 ± 2.00	K	NIST Webbook
tb	390.78 ± 0.30	K	NIST Webbook
tb	390.77 ± 0.20	K	NIST Webbook
tb	390.75 ± 0.50	K	NIST Webbook
tc	561.70 ± 0.50	K	NIST Webbook
tc	561.67 ± 0.40	K	NIST Webbook
tc	561.70	K	KDB
tc	561.70	K	NIST Webbook
tf	152.16 ± 0.01	K	NIST Webbook
tf	152.17 ± 0.05	K	NIST Webbook
tf	152.19 ± 0.03	K	NIST Webbook
tf	151.98 ± 0.30	K	NIST Webbook
tf	152.17 ± 0.06	K	NIST Webbook
tf	152.07 ± 0.15	K	NIST Webbook
tf	152.06 ± 0.20	K	NIST Webbook
tf	152.06 ± 0.30	K	NIST Webbook
tf	152.00	K	KDB

tf	148.85 ± 0.30	K	NIST Webbook
tf	148.85 ± 2.00	K	NIST Webbook
vc	0.476	m3/kmol	NIST Webbook
vc	0.476	m3/kmol	KDB
zc	0.2588810		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.46	J/mol×K	549.20	Joback Method
cpg	282.86	J/mol×K	493.46	Joback Method
cpg	270.88	J/mol×K	465.60	Joback Method
cpg	258.44	J/mol×K	437.73	Joback Method
cpg	245.53	J/mol×K	409.87	Joback Method
cpg	232.14	J/mol×K	382.00	Joback Method
cpg	294.38	J/mol×K	521.33	Joback Method
cpl	251.08	J/mol×K	298.15	NIST Webbook
dvisc	0.0031758	Pa×s	201.10	Joback Method
dvisc	0.0013776	Pa×s	237.28	Joback Method
dvisc	0.0007454	Pa×s	273.46	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	0.0105616	Pa×s	164.92	Joback Method
hfust	10.84	kJ/mol	152.20	NIST Webbook
hfust	10.84	kJ/mol	152.20	NIST Webbook
hvapt	38.70 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	38.20	kJ/mol	352.00	NIST Webbook
hvapt	33.35	kJ/mol	390.90	NIST Webbook
hvapt	42.30	kJ/mol	322.00	NIST Webbook
hvapt	36.10 ± 0.10	kJ/mol	353.00	NIST Webbook
hvapt	37.40 ± 0.10	kJ/mol	333.00	NIST Webbook
hvapt	33.89	kJ/mol	390.90	KDB
rfi	1.39553		298.15	KDB
rhol	705.00	kg/m3	293.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43890e+01
Coeff. B	-3.39289e+03
Coeff. C	-4.36080e+01
Temperature range (K), min.	284.21
Temperature range (K), max.	417.38

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.98808e+01
Coeff. B	-7.72965e+03
Coeff. C	-1.11685e+01
Coeff. D	7.67739e-06
Temperature range (K), min.	152.20
Temperature range (K), max.	561.74

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol49.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C589537&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=49
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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