3-Heptene, (E)-

Other names:	(E)-3-HEPTENE
	(E)-hept-3-ene
	3-C7H14
	TRANS-3-HEPTENE
Inchi:	InChI=1S/C7H14/c1-3-5-7-6-4-2/h5,7H,3-4,6H2,1-2H3/b7-5+
InchiKey:	WZHKDGJSXCTSCK-FNORWQNLSA-N
Formula:	C7H14
SMILES:	CCC=CCCC
Mol. weight [g/mol]:	98.19
CAS:	14686-14-7

Physical Properties

Property code	Value	Unit	Source
chl	-4646.04 ± 0.92	kJ/mol	NIST Webbook
gf	88.28	kJ/mol	Joback Method
hf	-73.50 ± 1.00	kJ/mol	NIST Webbook
hf	-74.10	kJ/mol	NIST Webbook
hf	-72.60 ± 0.70	kJ/mol	NIST Webbook
hf	-73.20	kJ/mol	NIST Webbook
hfl	-108.40 ± 0.63	kJ/mol	NIST Webbook
hfl	-109.30 ± 1.00	kJ/mol	NIST Webbook
hfus	14.09	kJ/mol	Joback Method
hvap	35.60	kJ/mol	NIST Webbook
ie	8.92	eV	NIST Webbook
log10ws	-2.61		Crippen Method
logp	2.753		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
rinpol	694.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	692.10		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	687.00		NIST Webbook

rinpol	687.00	NIST Webbook
rinpol	687.00	NIST Webbook
rinpol	688.00	NIST Webbook
rinpol	691.30	NIST Webbook
rinpol	687.50	NIST Webbook
rinpol	688.00	NIST Webbook
rinpol	687.40	NIST Webbook
rinpol	687.50	NIST Webbook
rinpol	690.00	NIST Webbook
rinpol	688.00	NIST Webbook
rinpol	688.00	NIST Webbook
rinpol	688.00	NIST Webbook
rinpol	688.00	NIST Webbook
rinpol	698.40	NIST Webbook
rinpol	697.90	NIST Webbook
rinpol	697.00	NIST Webbook
rinpol	697.50	NIST Webbook
rinpol	697.72	NIST Webbook
rinpol	698.00	NIST Webbook
rinpol	687.40	NIST Webbook
rinpol	688.00	NIST Webbook
rinpol	688.00	NIST Webbook
rinpol	688.00	NIST Webbook
rinpol	698.00	NIST Webbook
rinpol	698.00	NIST Webbook
rinpol	698.00	NIST Webbook
rinpol	696.00	NIST Webbook
rinpol	698.00	NIST Webbook
rinpol	687.00	NIST Webbook
rinpol	698.00	NIST Webbook
rinpol	698.00	NIST Webbook
rinpol	698.00	NIST Webbook
rinpol	687.40	NIST Webbook
rinpol	698.40	NIST Webbook
rinpol	697.90	NIST Webbook
rinpol	694.00	NIST Webbook
rinpol	687.50	NIST Webbook
rinpol	688.00	NIST Webbook
rinpol	698.00	NIST Webbook
rinpol	690.00	NIST Webbook
rinpol	698.00	NIST Webbook
rinpol	687.00	NIST Webbook
rinpol	698.00	NIST Webbook
rinpol	687.50	NIST Webbook

rinpol	687.50		NIST Webbook
rinpol	694.20		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	687.40		NIST Webbook
rinpol	698.40		NIST Webbook
rinpol	691.30		NIST Webbook
rinpol	687.60		NIST Webbook
ripol	735.00		NIST Webbook
ripol	752.00		NIST Webbook
ripol	750.00		NIST Webbook
ripol	746.00		NIST Webbook
ripol	748.00		NIST Webbook
ripol	749.00		NIST Webbook
ripol	747.70		NIST Webbook
ripol	746.40		NIST Webbook
ripol	749.00		NIST Webbook
ripol	746.40		NIST Webbook
ripol	752.00		NIST Webbook
ripol	749.00		NIST Webbook
ripol	735.00		NIST Webbook
ripol	714.00		NIST Webbook
ripol	747.70		NIST Webbook
ripol	747.70		NIST Webbook
ripol	749.00		NIST Webbook
ripol	714.00		NIST Webbook
tb	369.00 ± 2.00	K	NIST Webbook
tb	369.15 ± 1.00	K	NIST Webbook
tb	367.20	K	NIST Webbook
tb	368.90	K	NIST Webbook
tb	368.70 ± 1.00	K	NIST Webbook
tb	368.90 ± 1.00	K	NIST Webbook
tb	368.90 ± 1.00	K	NIST Webbook
tb	368.00 ± 2.00	K	NIST Webbook
tb	368.81 ± 0.20	K	NIST Webbook
tb	368.83 ± 0.20	K	NIST Webbook
tb	368.84 ± 0.30	K	NIST Webbook
tb	367.15 ± 2.00	K	NIST Webbook
tb	368.83 ± 0.30	K	NIST Webbook
tb	369.65 ± 2.00	K	NIST Webbook
tb	368.95 ± 1.00	K	NIST Webbook

tb	368.65 ± 2.00	K	NIST Webbook
tb	369.20 ± 1.00	K	NIST Webbook
tb	369.20 ± 1.00	K	NIST Webbook
tb	369.25 ± 1.00	K	NIST Webbook
tb	370.65 ± 2.00	K	NIST Webbook
tc	538.60	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	136.49 ± 0.06	K	NIST Webbook
tf	136.52 ± 0.04	K	NIST Webbook
tf	136.49 ± 0.06	K	NIST Webbook
tf	136.49 ± 0.06	K	NIST Webbook
tf	136.52 ± 0.04	K	NIST Webbook
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.32	J/mol×K	363.72	Joback Method
cpg	192.00	J/mol×K	392.43	Joback Method
cpg	203.19	J/mol×K	421.15	Joback Method
cpg	213.90	J/mol×K	449.86	Joback Method
cpg	224.15	J/mol×K	478.58	Joback Method
cpg	233.95	J/mol×K	507.29	Joback Method
cpg	243.33	J/mol×K	536.01	Joback Method
dvisc	0.0047393	Pa×s	163.57	Joback Method
dvisc	0.0017796	Pa×s	196.93	Joback Method
dvisc	0.0008875	Pa×s	230.29	Joback Method
dvisc	0.0005278	Pa×s	263.64	Joback Method
dvisc	0.0003528	Pa×s	297.00	Joback Method
dvisc	0.0002558	Pa×s	330.36	Joback Method
dvisc	0.0001967	Pa×s	363.72	Joback Method
hvapt	34.60	kJ/mol	340.00	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45052e+01
Coeff. B	-3.32231e+03
Coeff. C	-3.27880e+01
Temperature range (K), min.	266.46
Temperature range (K), max.	394.15

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.95241e+01
Coeff. B	-7.41197e+03
Coeff. C	-1.29776e+01
Coeff. D	1.38838e-05
Temperature range (K), min.	268.15
Temperature range (K), max.	394.15

Sources

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=217

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=217

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14686147&Units=SI

Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons: https://www.doi.org/10.1021/je0341357

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

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

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfl: Liquid phase enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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