(Z)-2-Heptene

Other names:	(Z)-2-C7H14
	(Z)-hept-2-ene
	2-Heptene, (Z)-
	CIS-2-HEPTENE
Inchi:	InChI=1S/C7H14/c1-3-5-7-6-4-2/h3,5H,4,6-7H2,1-2H3/b5-3-
InchiKey:	OTTZHAVKAVGASB-HYXAFXHYSA-N
Formula:	C7H14
SMILES:	CC=CCCCC
Mol. weight [g/mol]:	98.19
CAS:	6443-92-1

Physical Properties

Property code	Value	Unit	Source
chl	-4650.22 ± 0.79	kJ/mol	NIST Webbook
gf	88.28	kJ/mol	Joback Method
hf	-70.70	kJ/mol	NIST Webbook
hf	-68.80 ± 1.00	kJ/mol	NIST Webbook
hf	-69.90	kJ/mol	NIST Webbook
hf	-69.60 ± 0.70	kJ/mol	NIST Webbook
hfl	-105.90 ± 0.63	kJ/mol	NIST Webbook
hfl	-105.10 ± 0.92	kJ/mol	NIST Webbook
hfus	14.09	kJ/mol	Joback Method
hvap	36.00	kJ/mol	NIST Webbook
hvap	38.60	kJ/mol	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	704.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	709.00		NIST Webbook
rinpol	713.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	714.00		NIST Webbook
rinpol	702.40		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	712.10		NIST Webbook

rinpol	712.20	NIST Webbook
rinpol	713.20	NIST Webbook
rinpol	710.00	NIST Webbook
rinpol	710.93	NIST Webbook
rinpol	710.92	NIST Webbook
rinpol	714.40	NIST Webbook
rinpol	708.80	NIST Webbook
rinpol	704.00	NIST Webbook
rinpol	711.00	NIST Webbook
rinpol	705.00	NIST Webbook
rinpol	713.00	NIST Webbook
rinpol	704.00	NIST Webbook
rinpol	709.00	NIST Webbook
rinpol	715.00	NIST Webbook
rinpol	700.00	NIST Webbook
rinpol	702.40	NIST Webbook
rinpol	708.80	NIST Webbook
rinpol	705.00	NIST Webbook
rinpol	711.00	NIST Webbook
rinpol	714.40	NIST Webbook
rinpol	712.80	NIST Webbook
rinpol	702.10	NIST Webbook
rinpol	705.00	NIST Webbook
rinpol	712.00	NIST Webbook
rinpol	713.00	NIST Webbook
rinpol	713.00	NIST Webbook
rinpol	713.00	NIST Webbook
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rinpol	712.00	NIST Webbook
rinpol	712.00	NIST Webbook
rinpol	705.90	NIST Webbook
rinpol	704.00	NIST Webbook
rinpol	700.40	NIST Webbook
rinpol	704.40	NIST Webbook
rinpol	705.00	NIST Webbook
rinpol	705.00	NIST Webbook
rinpol	704.00	NIST Webbook
rinpol	713.20	NIST Webbook
rinpol	703.50	NIST Webbook
rinpol	704.00	NIST Webbook
rinpol	705.10	NIST Webbook
rinpol	704.30	NIST Webbook
rinpol	700.00	NIST Webbook

rinpol	703.00		NIST Webbook
rinpol	712.20		NIST Webbook
ripol	790.00		NIST Webbook
ripol	760.00		NIST Webbook
ripol	760.00		NIST Webbook
ripol	784.00		NIST Webbook
ripol	783.80		NIST Webbook
ripol	778.90		NIST Webbook
ripol	778.70		NIST Webbook
ripol	783.80		NIST Webbook
ripol	786.00		NIST Webbook
ripol	778.90		NIST Webbook
ripol	784.00		NIST Webbook
ripol	781.00		NIST Webbook
ripol	779.00		NIST Webbook
ripol	778.70		NIST Webbook
tb	371.40 ± 0.50	K	NIST Webbook
tb	371.70	K	NIST Webbook
tb	371.65 ± 2.00	K	NIST Webbook
tb	372.25 ± 2.00	K	NIST Webbook
tb	372.25 ± 1.00	K	NIST Webbook
tb	372.15 ± 1.00	K	NIST Webbook
tb	370.75 ± 1.00	K	NIST Webbook
tb	371.40 ± 0.70	K	NIST Webbook
tb	369.15 ± 2.00	K	NIST Webbook
tb	371.40 ± 1.00	K	NIST Webbook
tb	371.56 ± 0.30	K	NIST Webbook
tb	371.80 ± 0.20	K	NIST Webbook
tc	548.50	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	163.57	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.95	J/mol×K	507.29	Joback Method
cpg	213.90	J/mol×K	449.86	Joback Method
cpg	203.19	J/mol×K	421.15	Joback Method
cpg	192.00	J/mol×K	392.43	Joback Method

cpg	180.32	J/mol×K	363.72	Joback Method
cpg	224.15	J/mol×K	478.58	Joback Method
cpg	243.33	J/mol×K	536.01	Joback Method
dvisc	0.0047393	Pa×s	163.57	Joback Method
dvisc	0.0001967	Pa×s	363.72	Joback Method
dvisc	0.0002558	Pa×s	330.36	Joback Method
dvisc	0.0003528	Pa×s	297.00	Joback Method
dvisc	0.0005278	Pa×s	263.64	Joback Method
dvisc	0.0008875	Pa×s	230.29	Joback Method
dvisc	0.0017796	Pa×s	196.93	Joback Method
hvapt	34.60	kJ/mol	351.50	NIST Webbook
hvapt	39.00 ± 0.30	kJ/mol	290.00	NIST Webbook
hvapt	35.30	kJ/mol	343.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42449e+01
Coeff. B	-3.22507e+03
Coeff. C	-3.65420e+01
Temperature range (K), min.	267.61
Temperature range (K), max.	397.55

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.88865e+01
Coeff. B	-6.04816e+03
Coeff. C	-6.50618e+00
Coeff. D	3.65600e-06
Temperature range (K), min.	164.00
Temperature range (K), max.	549.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=214
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=214
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6443921&Units=SI

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
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