2-Hexene, (Z)-

Other names: (Z)-2-C6H12
(Z)-2-HEXENE
(Z)-hex-2-ene
2-Hexene, cis-
CIS-2-HEXENE
Inchi: InChI=1S/C6H12/c1-3-5-6-4-2/h3,5H,4,6H2,1-2H3/b5-3-
InchiKey: RYPKRALMXUUNKS-HYXAFXHYSA-N
Formula: C6H12
SMILES: CC=CCCC
Mol. weight [g/mol]: 84.16
CAS: 7688-21-3

Physical Properties

Property code	Value	Unit	Source
af	0.2560		KDB
ap	299.150	K	KDB
gf	76.28	kJ/mol	KDB
hcg	3992.20	kJ/mol	KDB
hcn	3728.111	kJ/mol	KDB
hf	-47.50 ± 1.10	kJ/mol	NIST Webbook
hf	-49.40	kJ/mol	NIST Webbook
hf	-47.90 ± 1.00	kJ/mol	NIST Webbook
hf	-47.00 ± 1.10	kJ/mol	NIST Webbook
hf	-53.30 ± 1.20	kJ/mol	NIST Webbook
hf	-52.38	kJ/mol	KDB
hfl	-79.20 ± 1.00	kJ/mol	NIST Webbook
hfl	-79.70 ± 1.00	kJ/mol	NIST Webbook
hfl	-85.50 ± 1.10	kJ/mol	NIST Webbook
hfl	-80.12 ± 0.84	kJ/mol	NIST Webbook
hfus	11.50	kJ/mol	Joback Method
hvap	31.50	kJ/mol	NIST Webbook
hvap	31.50	kJ/mol	NIST Webbook
hvap	31.50	kJ/mol	NIST Webbook
ie	8.97 ± 0.01	eV	NIST Webbook
ie	8.97 ± 0.01	eV	NIST Webbook
ie	9.15 ± 0.01	eV	NIST Webbook
log10ws	-2.19		Crippen Method

logp	2.363		Crippen Method
mcvol	91.100	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
pc	3280.00	kPa	KDB
rinpol	603.60		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	613.60		NIST Webbook
rinpol	614.30		NIST Webbook
rinpol	613.00		NIST Webbook
rinpol	604.60		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	603.60		NIST Webbook
rinpol	604.20		NIST Webbook
rinpol	604.00		NIST Webbook
rinpol	604.00		NIST Webbook
rinpol	602.40		NIST Webbook
rinpol	604.00		NIST Webbook
rinpol	604.00		NIST Webbook
rinpol	602.52		NIST Webbook
rinpol	605.00		NIST Webbook
rinpol	605.00		NIST Webbook
rinpol	605.00		NIST Webbook
rinpol	616.10		NIST Webbook
rinpol	605.00		NIST Webbook
rinpol	604.00		NIST Webbook
rinpol	605.40		NIST Webbook
rinpol	604.60		NIST Webbook
rinpol	600.00		NIST Webbook
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rinpol	604.00		NIST Webbook
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rinpol	606.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	614.75		NIST Webbook
rinpol	616.00		NIST Webbook
rinpol	614.50		NIST Webbook
rinpol	610.48		NIST Webbook
rinpol	610.48		NIST Webbook
rinpol	602.70		NIST Webbook

rinpol	616.00		NIST Webbook
rinpol	603.10		NIST Webbook
rinpol	604.00		NIST Webbook
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rinpol	615.00		NIST Webbook
rinpol	604.20		NIST Webbook
rinpol	604.00		NIST Webbook
rinpol	616.10		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	614.50		NIST Webbook
rinpol	603.10		NIST Webbook
rinpol	616.00		NIST Webbook
rinpol	604.00		NIST Webbook
rinpol	613.00		NIST Webbook
rinpol	610.00		NIST Webbook
ripol	680.00		NIST Webbook
ripol	680.00		NIST Webbook
ripol	680.00		NIST Webbook
ripol	679.80		NIST Webbook
ripol	679.80		NIST Webbook
ripol	680.50		NIST Webbook
ripol	680.50		NIST Webbook
ripol	679.80		NIST Webbook
sl	291.86	J/mol×K	NIST Webbook

tb	341.85 ± 0.40	K	NIST Webbook
tb	342.05 ± 0.40	K	NIST Webbook
tb	342.01 ± 0.20	K	NIST Webbook
tb	342.00 ± 0.40	K	NIST Webbook
tb	342.00	K	NIST Webbook
tb	341.94 ± 0.60	K	NIST Webbook
tb	342.00	K	KDB
tb	342.15 ± 1.00	K	NIST Webbook
tb	342.03 ± 0.50	K	NIST Webbook
tc	518.00	K	KDB
tc	513.40	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	128.65 ± 1.00	K	NIST Webbook
tf	127.15 ± 1.50	K	NIST Webbook
tf	129.03 ± 0.70	K	NIST Webbook
tf	131.77 ± 0.15	K	NIST Webbook
tf	131.35 ± 1.00	K	NIST Webbook
tf	132.00	K	KDB
tf	129.99 ± 2.00	K	NIST Webbook
tt	132.03 ± 0.00	K	NIST Webbook
vc	0.351	m3/kmol	KDB
zc	0.2673100		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.78	J/mol×K	513.19	Joback Method
cpg	183.82	J/mol×K	455.74	Joback Method
cpg	174.75	J/mol×K	427.01	Joback Method
cpg	165.27	J/mol×K	398.29	Joback Method
cpg	155.37	J/mol×K	369.56	Joback Method
cpg	145.03	J/mol×K	340.84	Joback Method
cpg	192.49	J/mol×K	484.46	Joback Method
cpl	178.36	J/mol×K	298.15	NIST Webbook
dvisc	0.0015745	Pa×s	183.72	Joback Method
dvisc	0.0002395	Pa×s	309.42	Joback Method
dvisc	0.0001858	Pa×s	340.84	Joback Method
dvisc	0.0004831	Pa×s	246.57	Joback Method
dvisc	0.0040974	Pa×s	152.30	Joback Method
dvisc	0.0003269	Pa×s	277.99	Joback Method

dvisc	0.0008000	Pa×s	215.15	Joback Method
hfust	8.88	kJ/mol	132.03	NIST Webbook
hfust	8.88	kJ/mol	132.00	NIST Webbook
hfust	8.88	kJ/mol	132.00	NIST Webbook
hvapt	32.20	kJ/mol	310.50	NIST Webbook
hvapt	29.12	kJ/mol	342.00	KDB
rfi	1.39473		298.15	KDB
rhol	687.00	kg/m3	293.00	KDB
sfust	67.24	J/mol×K	132.03	NIST Webbook
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43327e+01
Coeff. B	-3.02937e+03
Coeff. C	-3.01870e+01
Temperature range (K), min.	245.88
Temperature range (K), max.	365.99

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.77937e+01
Coeff. B	-5.52489e+03
Coeff. C	-6.43715e+00
Coeff. D	4.59912e-06
Temperature range (K), min.	132.00
Temperature range (K), max.	513.00

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=197

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

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

Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=197
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7688213&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
ap:	Aniline Point
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

vc: Critical Volume

zc: Critical Compressibility