2-Hexene, (E)-

Other names:	(E)-2-C6H12
	(E)-2-HEXENE
	TRANS-2-HEXENE
	trans-hex-2-ene
Inchi:	InChI=1S/C6H12/c1-3-5-6-4-2/h3,5H,4,6H2,1-2H3/b5-3+
InchiKey:	RYPKRALMXUUNKS-HWKANZROSA-N
Formula:	C6H12
SMILES:	CC=CCCC
Mol. weight [g/mol]:	84.16
CAS:	4050-45-7

Physical Properties

Property code	Value	Unit	Source
af	0.2420		KDB
ap	299.150	K	KDB
gf	76.49	kJ/mol	KDB
hcg	3990.57	kJ/mol	KDB
hcn	3726.480	kJ/mol	KDB
hf	-52.10 ± 1.00	kJ/mol	NIST Webbook
hf	-52.50	kJ/mol	NIST Webbook
hf	-51.60 ± 0.80	kJ/mol	NIST Webbook
hf	-51.00 ± 0.80	kJ/mol	NIST Webbook
hf	-53.93	kJ/mol	KDB
hf	-55.80 ± 1.30	kJ/mol	NIST Webbook
hfl	-82.60 ± 0.80	kJ/mol	NIST Webbook
hfl	-87.40 ± 1.30	kJ/mol	NIST Webbook
hfl	-83.22 ± 0.84	kJ/mol	NIST Webbook
hfl	-83.70 ± 1.00	kJ/mol	NIST Webbook
hfus	11.50	kJ/mol	Joback Method
hvap	32.20	kJ/mol	NIST Webbook
hvap	31.50	kJ/mol	NIST Webbook
hvap	31.50	kJ/mol	NIST Webbook
hvap	31.60	kJ/mol	NIST Webbook
ie	8.97 ± 0.01	eV	NIST Webbook
ie	9.16 ± 0.01	eV	NIST Webbook
ie	8.93	eV	NIST Webbook
ie	8.97 ± 0.02	eV	NIST Webbook

log10ws	-2.19		Crippen Method
logp	2.363		Crippen Method
mcvol	91.100	ml/mol	McGowan Method
pc	3270.00	kPa	KDB
rinpol	605.50		NIST Webbook
rinpol	597.00		NIST Webbook
rinpol	596.60		NIST Webbook
rinpol	597.00		NIST Webbook
rinpol	597.00		NIST Webbook
rinpol	597.30		NIST Webbook
rinpol	597.00		NIST Webbook
rinpol	597.00		NIST Webbook
rinpol	596.60		NIST Webbook
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rinpol	603.38		NIST Webbook
rinpol	603.43		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	604.00		NIST Webbook
rinpol	596.90		NIST Webbook
rinpol	597.00		NIST Webbook
rinpol	598.00		NIST Webbook
rinpol	613.00		NIST Webbook
rinpol	605.00		NIST Webbook
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rinpol	604.90	NIST Webbook
rinpol	596.60	NIST Webbook
rinpol	596.00	NIST Webbook
rinpol	606.00	NIST Webbook
ripol	663.40	NIST Webbook
ripol	663.40	NIST Webbook
ripol	663.00	NIST Webbook

ripol	648.00		NIST Webbook
ripol	660.00		NIST Webbook
ripol	663.40		NIST Webbook
ripol	663.40		NIST Webbook
ripol	663.00		NIST Webbook
ripol	663.00		NIST Webbook
ripol	663.40		NIST Webbook
tb	340.27 ± 0.40	K	NIST Webbook
tb	341.06 ± 0.30	K	NIST Webbook
tb	339.15 ± 2.00	K	NIST Webbook
tb	341.02 ± 0.30	K	NIST Webbook
tb	341.00	K	KDB
tb	340.24 ± 0.20	K	NIST Webbook
tb	341.10 ± 0.40	K	NIST Webbook
tb	341.06 ± 0.40	K	NIST Webbook
tb	341.10	K	NIST Webbook
tb	341.25 ± 0.50	K	NIST Webbook
tb	341.23 ± 0.30	K	NIST Webbook
tb	341.23 ± 0.50	K	NIST Webbook
tb	341.23 ± 0.40	K	NIST Webbook
tb	340.28 ± 0.30	K	NIST Webbook
tc	516.00	K	KDB
tc	509.00	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	139.75 ± 0.60	K	NIST Webbook
tf	140.00	K	KDB
tf	140.17 ± 0.04	K	NIST Webbook
tf	140.08 ± 0.20	K	NIST Webbook
tf	139.75 ± 0.40	K	NIST Webbook
tf	139.65 ± 1.50	K	NIST Webbook
tf	139.99 ± 0.40	K	NIST Webbook
vc	0.351	m3/kmol	KDB
zc	0.2675280		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.78	J/mol×K	513.19	Joback Method
cpg	145.03	J/mol×K	340.84	Joback Method
cpg	155.37	J/mol×K	369.56	Joback Method

cpg	165.27	J/mol×K	398.29	Joback Method
cpg	174.75	J/mol×K	427.01	Joback Method
cpg	183.82	J/mol×K	455.74	Joback Method
cpg	192.49	J/mol×K	484.46	Joback Method
dvisc	0.0001858	Pa×s	340.84	Joback Method
dvisc	0.0040974	Pa×s	152.30	Joback Method
dvisc	0.0015745	Pa×s	183.72	Joback Method
dvisc	0.0008000	Pa×s	215.15	Joback Method
dvisc	0.0004831	Pa×s	246.57	Joback Method
dvisc	0.0003269	Pa×s	277.99	Joback Method
dvisc	0.0002395	Pa×s	309.42	Joback Method
hvapt	28.91	kJ/mol	341.00	KDB
rfi	1.39073		298.15	KDB
rhol	678.00	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	1.41268e+01
Coeff. B	-2.88478e+03
Coeff. C	-3.76300e+01
Temperature range (K), min.	246.08
Temperature range (K), max.	364.88

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.51774e+01
Coeff. B	-6.19923e+03
Coeff. C	-9.12514e+00
Coeff. D	7.24225e-06
Temperature range (K), min.	140.17
Temperature range (K), max.	513.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=198
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=198
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4050457&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
ap:	Aniline Point
cpg:	Ideal gas 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
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
rfi:	Refractive Index
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