3-Hexene, (Z)-

Other names: (Z)-3-C6H12
(Z)-3-HEXENE
CIS-3-HEXENE
Inchi: InChI=1S/C6H12/c1-3-5-6-4-2/h5-6H,3-4H2,1-2H3/b6-5-
InchiKey: ZQDPJFUHLCOCRG-WAYWQWQTSA-N
Formula: C6H12
SMILES: CCC=CCC
Mol. weight [g/mol]: 84.16
CAS: 7642-09-3

Physical Properties

Property code	Value	Unit	Source
af	0.2250		KDB
ap	300.150	K	KDB
dm	0.30	debye	KDB
gf	83.07	kJ/mol	KDB
hcg	3997.18	kJ/mol	KDB
hcn	3733.090	kJ/mol	KDB
hf	-48.00 ± 1.40	kJ/mol	NIST Webbook
hf	-48.20 ± 1.40	kJ/mol	NIST Webbook
hf	-47.40	kJ/mol	NIST Webbook
hf	-47.65	kJ/mol	KDB
hf	-45.90 ± 0.70	kJ/mol	NIST Webbook
hf	-46.90 ± 0.80	kJ/mol	NIST Webbook
hfl	-79.20 ± 1.40	kJ/mol	NIST Webbook
hfl	-78.07 ± 0.84	kJ/mol	NIST Webbook
hfl	-77.10 ± 0.70	kJ/mol	NIST Webbook
hfl	-79.40 ± 1.40	kJ/mol	NIST Webbook
hfus	11.50	kJ/mol	Joback Method
hvap	31.30	kJ/mol	NIST Webbook
hvap	31.30	kJ/mol	NIST Webbook
hvap	31.30	kJ/mol	NIST Webbook
hvap	31.30	kJ/mol	NIST Webbook
ie	9.15 ± 0.01	eV	NIST Webbook
ie	8.95 ± 0.01	eV	NIST Webbook
log10ws	-2.19		Crippen Method
logp	2.363		Crippen Method

mcvol	91.100	ml/mol	McGowan Method
pc	3280.00	kPa	KDB
rinpol	602.28		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	604.00		NIST Webbook
rinpol	593.00		NIST Webbook
rinpol	592.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	593.00		NIST Webbook
rinpol	604.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	602.20		NIST Webbook
rinpol	592.10		NIST Webbook
rinpol	593.00		NIST Webbook
rinpol	593.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	602.40		NIST Webbook
rinpol	602.70		NIST Webbook
rinpol	592.80		NIST Webbook
rinpol	593.10		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	603.00		NIST Webbook
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rinpol	607.90		NIST Webbook
rinpol	607.90		NIST Webbook
rinpol	607.90		NIST Webbook
rinpol	607.90		NIST Webbook
rinpol	602.30		NIST Webbook
rinpol	602.90		NIST Webbook
rinpol	603.50		NIST Webbook
rinpol	604.20		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	605.60		NIST Webbook

rinpol	604.80		NIST Webbook
rinpol	604.50		NIST Webbook
rinpol	603.60		NIST Webbook
rinpol	602.90		NIST Webbook
rinpol	602.20		NIST Webbook
rinpol	601.40		NIST Webbook
rinpol	593.00		NIST Webbook
rinpol	593.00		NIST Webbook
rinpol	592.20		NIST Webbook
rinpol	593.00		NIST Webbook
rinpol	593.00		NIST Webbook
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rinpol	593.00		NIST Webbook
rinpol	594.00		NIST Webbook
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rinpol	594.00		NIST Webbook
rinpol	593.00		NIST Webbook
rinpol	593.00		NIST Webbook
rinpol	603.75		NIST Webbook
rinpol	604.00		NIST Webbook
rinpol	601.60		NIST Webbook
rinpol	602.19		NIST Webbook
rinpol	604.90		NIST Webbook
rinpol	592.20		NIST Webbook
ripol	660.00		NIST Webbook
ripol	660.10		NIST Webbook
ripol	660.10		NIST Webbook
ripol	660.10		NIST Webbook
ripol	660.10		NIST Webbook
ripol	660.00		NIST Webbook
tb	339.79 ± 0.50	K	NIST Webbook
tb	339.71 ± 0.50	K	NIST Webbook
tb	339.66 ± 0.20	K	NIST Webbook
tb	339.79 ± 0.30	K	NIST Webbook
tb	339.65 ± 0.50	K	NIST Webbook

tb	339.63 ± 0.30	K	NIST Webbook
tb	339.60 ± 0.40	K	NIST Webbook
tb	339.60	K	NIST Webbook
tb	339.60	K	KDB
tb	343.80 ± 1.50	K	NIST Webbook
tb	339.70 ± 0.50	K	NIST Webbook
tb	339.80 ± 0.30	K	NIST Webbook
tb	340.15 ± 0.30	K	NIST Webbook
tb	339.67 ± 0.20	K	NIST Webbook
tb	340.05 ± 0.20	K	NIST Webbook
tc	510.20	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tc	517.00	K	KDB
tf	133.51 ± 0.50	K	NIST Webbook
tf	134.70 ± 1.00	K	NIST Webbook
tf	138.15 ± 1.50	K	NIST Webbook
tf	135.30	K	KDB
tf	134.85 ± 0.30	K	NIST Webbook
tf	135.27 ± 0.20	K	NIST Webbook
tf	134.70 ± 1.00	K	NIST Webbook
tf	138.00 ± 2.00	K	NIST Webbook
vc	0.350	m3/kmol	KDB
zc	0.2670640		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	200.78	J/mol×K	513.19	Joback Method
dvisc	0.0001858	Pa×s	340.84	Joback Method
dvisc	0.0015745	Pa×s	183.72	Joback Method
dvisc	0.0040974	Pa×s	152.30	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

dvisc	0.0008000	Pa×s	215.15	Joback Method
hvapt	28.70	kJ/mol	339.60	KDB
hvapt	32.10	kJ/mol	312.00	NIST Webbook
rfi	1.39189		298.15	KDB
rhol	680.00	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	1.42675e+01
Coeff. B	-2.94621e+03
Coeff. C	-3.42680e+01
Temperature range (K), min.	245.01
Temperature range (K), max.	363.23

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.26231e+01
Coeff. B	-6.03782e+03
Coeff. C	-8.76722e+00
Coeff. D	7.50792e-06
Temperature range (K), min.	135.33
Temperature range (K), max.	509.00

Sources

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

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

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=199

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=199

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

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

Legend

af:	Acentric Factor
ap:	Aniline Point
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
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