1-Hexene, 2-methyl-

Other names:	2-Methyl-1-hexene
	2-methylhex-1-ene
	n-C4H9C(CH3)=CH2
Inchi:	InChI=1S/C7H14/c1-4-5-6-7(2)3/h2,4-6H2,1,3H3
InchiKey:	IRUDSQHLKGNCGF-UHFFFAOYSA-N
Formula:	C7H14
SMILES:	C=C(C)CCCC
Mol. weight [g/mol]:	98.19
CAS:	6094-02-6

Physical Properties

Property code	Value	Unit	Source
gf	87.35	kJ/mol	Joback Method
hf	-72.17	kJ/mol	Joback Method
hfus	11.30	kJ/mol	Joback Method
hvap	35.10	kJ/mol	NIST Webbook
ie	9.04 ± 0.01	eV	NIST Webbook
log10ws	-2.61		Crippen Method
logp	2.753		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2944.08	kPa	Joback Method
rinpol	677.60		NIST Webbook
rinpol	679.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	677.50		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	686.80		NIST Webbook
rinpol	682.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	677.00		NIST Webbook
rinpol	679.00		NIST Webbook
rinpol	686.00		NIST Webbook

rinpol	686.00		NIST Webbook
rinpol	682.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	679.00		NIST Webbook
rinpol	685.90		NIST Webbook
rinpol	677.40		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	685.10		NIST Webbook
rinpol	685.80		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	676.70		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	678.10		NIST Webbook
rinpol	678.10		NIST Webbook
rinpol	677.50		NIST Webbook
rinpol	678.20		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	680.70		NIST Webbook
rinpol	678.10		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	677.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	679.00		NIST Webbook
rinpol	679.00		NIST Webbook
rinpol	679.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	686.80		NIST Webbook
rinpol	682.00		NIST Webbook
rinpol	685.90		NIST Webbook
ripol	735.00		NIST Webbook
ripol	740.00		NIST Webbook
ripol	740.00		NIST Webbook
ripol	723.00		NIST Webbook
ripol	735.00		NIST Webbook
tb	364.15 ± 1.00	K	NIST Webbook
tb	364.65 ± 1.00	K	NIST Webbook

tb	364.99 ± 0.30	K	NIST Webbook
tb	364.65 ± 0.50	K	NIST Webbook
tb	365.15 ± 0.20	K	NIST Webbook
tb	364.95 ± 0.30	K	NIST Webbook
tb	364.45 ± 1.00	K	NIST Webbook
tb	365.20	K	NIST Webbook
tb	364.15 ± 1.50	K	NIST Webbook
tb	364.45 ± 0.70	K	NIST Webbook
tb	366.30 ± 1.00	K	NIST Webbook
tb	365.16 ± 0.20	K	NIST Webbook
tc	541.80	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	170.31 ± 0.03	K	NIST Webbook
tf	170.29 ± 0.03	K	NIST Webbook
tf	170.31 ± 0.02	K	NIST Webbook
tf	170.29 ± 0.05	K	NIST Webbook
tf	170.28 ± 0.04	K	NIST Webbook
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.42	J/mol×K	498.05	Joback Method
cpg	180.52	J/mol×K	356.12	Joback Method
cpg	191.97	J/mol×K	384.51	Joback Method
cpg	202.97	J/mol×K	412.89	Joback Method
cpg	213.54	J/mol×K	441.28	Joback Method
cpg	223.68	J/mol×K	469.66	Joback Method
cpg	242.76	J/mol×K	526.43	Joback Method
hvapt	33.90	kJ/mol	354.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42414e+01

Coeff. B	-3.12657e+03
Coeff. C	-4.00860e+01
Temperature range (K), min.	264.15
Temperature range (K), max.	390.21

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.08369e+01
Coeff. B	-6.43223e+03
Coeff. C	-8.37143e+00
Coeff. D	5.94029e-06
Temperature range (K), min.	170.28
Temperature range (K), max.	538.00

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol218.mol
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=218
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6094026&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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