2-Hexene, 2-methyl-

Other names:	2-Methyl-2-hexene
	C3H7CH=C(CH3)2
Inchi:	InChI=1S/C7H14/c1-4-5-6-7(2)3/h6H,4-5H2,1-3H3
InchiKey:	BWEKDYGHDCHWEN-UHFFFAOYSA-N
Formula:	C7H14
SMILES:	CCCC=C(C)C
Mol. weight [g/mol]:	98.19
CAS:	2738-19-4

Physical Properties

Property code	Value	Unit	Source
gf	79.73	kJ/mol	Joback Method
hf	-80.38	kJ/mol	Joback Method
hfus	12.78	kJ/mol	Joback Method
hvap	35.60	kJ/mol	NIST Webbook
ie	8.62	eV	NIST Webbook
log10ws	-2.61		Crippen Method
logp	2.753		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	692.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	698.30		NIST Webbook
rinpol	698.30		NIST Webbook
rinpol	691.40		NIST Webbook
rinpol	691.40		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	694.10		NIST Webbook
rinpol	695.30		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	689.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	692.00		NIST Webbook

rinpol	692.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	690.50		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	701.35		NIST Webbook
rinpol	702.40		NIST Webbook
rinpol	691.20		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	697.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	699.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	701.35		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	702.40		NIST Webbook
rinpol	702.40		NIST Webbook
rinpol	698.00		NIST Webbook
tb	367.65 ± 0.50	K	NIST Webbook
tb	366.65 ± 3.00	K	NIST Webbook
tb	368.40 ± 1.00	K	NIST Webbook
tb	368.60	K	NIST Webbook
tb	368.65 ± 0.50	K	NIST Webbook
tb	366.60 ± 1.00	K	NIST Webbook
tb	368.58 ± 0.20	K	NIST Webbook
tb	368.56 ± 0.30	K	NIST Webbook
tb	368.25 ± 0.50	K	NIST Webbook
tb	367.15 ± 2.00	K	NIST Webbook
tb	368.58 ± 0.20	K	NIST Webbook

tb	367.35 ± 0.50	K	NIST Webbook
tb	368.56 ± 0.30	K	NIST Webbook
tb	368.56 ± 0.30	K	NIST Webbook
tb	367.70 ± 0.50	K	NIST Webbook
tb	368.25 ± 1.00	K	NIST Webbook
tc	539.41	K	Joback Method
tf	142.80 ± 0.03	K	NIST Webbook
tf	142.80 ± 0.03	K	NIST Webbook
tf	142.77 ± 0.04	K	NIST Webbook
tf	142.77 ± 0.04	K	NIST Webbook
tf	142.77 ± 0.05	K	NIST Webbook
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.79	J/mol×K	510.11	Joback Method
cpg	180.34	J/mol×K	363.60	Joback Method
cpg	192.22	J/mol×K	392.90	Joback Method
cpg	203.59	J/mol×K	422.20	Joback Method
cpg	214.47	J/mol×K	451.50	Joback Method
cpg	224.86	J/mol×K	480.80	Joback Method
cpg	244.29	J/mol×K	539.41	Joback Method
hvapt	34.00	kJ/mol	358.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42426e+01
Coeff. B	-3.16845e+03
Coeff. C	-3.93440e+01
Temperature range (K), min.	266.39
Temperature range (K), max.	394.11

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.21511e+01
Coeff. B	-7.24858e+03
Coeff. C	-1.17214e+01
Coeff. D	1.03268e-05
Temperature range (K), min.	267.15
Temperature range (K), max.	393.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2738194&Units=SI
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=222
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol222.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume