3-Hexene, 2-methyl-, (E)-

Other names:	(E)-2-METHYL-3-HEXENE
	(E)-2-methylhex-3-ene
	(E)-3-Hexene, 2-methyl
	2-METHYL-TRANS-3-HEXENE
	2-Methyl-3-hexene, trans
	TRANS-2-METHYL-3-HEXENE
Inchi:	InChI=1S/C7H14/c1-4-5-6-7(2)3/h5-7H,4H2,1-3H3/b6-5+
InchiKey:	IQANHWBWTVLDTP-AATRIKPKSA-N
Formula:	C7H14
SMILES:	CCC=CC(C)C
Mol. weight [g/mol]:	98.19
CAS:	692-24-0

Physical Properties

Property code	Value	Unit	Source
gf	85.84	kJ/mol	Joback Method
hf	-75.87	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	34.30	kJ/mol	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.609		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
rinpol	647.00		NIST Webbook
rinpol	649.10		NIST Webbook
rinpol	649.40		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	656.00		NIST Webbook
rinpol	648.00		NIST Webbook
rinpol	648.00		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	648.00		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	661.00		NIST Webbook

rinpol	660.00		NIST Webbook
rinpol	661.10		NIST Webbook
rinpol	647.20		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	651.00		NIST Webbook
rinpol	656.00		NIST Webbook
rinpol	661.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	647.40		NIST Webbook
rinpol	660.50		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	664.00		NIST Webbook
tb	367.10 ± 0.50	K	NIST Webbook
tb	359.07 ± 0.30	K	NIST Webbook
tb	359.07 ± 0.30	K	NIST Webbook
tb	359.10	K	NIST Webbook
tb	359.02 ± 0.20	K	NIST Webbook
tc	539.72	K	Joback Method
tf	148.57	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.01	J/mol×K	539.72	Joback Method
cpg	180.16	J/mol×K	363.28	Joback Method
cpg	192.22	J/mol×K	392.69	Joback Method
cpg	203.76	J/mol×K	422.09	Joback Method
cpg	214.79	J/mol×K	451.50	Joback Method
cpg	225.33	J/mol×K	480.91	Joback Method
cpg	235.39	J/mol×K	510.31	Joback Method
dvisc	0.0001915	Pa×s	363.28	Joback Method
dvisc	0.0095853	Pa×s	148.57	Joback Method
dvisc	0.0026515	Pa×s	184.35	Joback Method
dvisc	0.0011138	Pa×s	220.14	Joback Method
dvisc	0.0005963	Pa×s	255.92	Joback Method
dvisc	0.0003722	Pa×s	291.71	Joback Method
dvisc	0.0002575	Pa×s	327.50	Joback Method

hvapt	33.50	kJ/mol	348.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39948e+01
Coeff. B	-2.89637e+03
Coeff. C	-5.01530e+01
Temperature range (K), min.	261.46
Temperature range (K), max.	383.71

Sources

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/research/kdb/hcprop/showprop.php?cmpid=230

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C692240&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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

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