2-Hexene, 4-methyl-, (E)-

Other names:	(E)-4-METHYL-2-HEXENE
	(E)-C2H5CH(CH3)CH=CHCH3
	4-METHYL-TRANS-2-HEXENE
	4-Methyl-2-hexene (trans)
	TRANS-4-METHYL-2-HEXENE
Inchi:	InChI=1S/C7H14/c1-4-6-7(3)5-2/h4,6-7H,5H2,1-3H3/b6-4+
InchiKey:	MBNDKEPQUVZHCM-GQCTYLIASA-N
Formula:	C7H14
SMILES:	CC=CC(C)CC
Mol. weight [g/mol]:	98.19
CAS:	3683-22-5

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	34.70	kJ/mol	NIST Webbook
hvap	34.70	kJ/mol	NIST Webbook
ie	8.91 ± 0.01	eV	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	658.00		NIST Webbook
rinpol	666.00		NIST Webbook
rinpol	666.00		NIST Webbook
rinpol	657.40		NIST Webbook
rinpol	657.50		NIST Webbook
rinpol	657.00		NIST Webbook
rinpol	659.20		NIST Webbook
rinpol	662.00		NIST Webbook
rinpol	662.00		NIST Webbook
rinpol	657.00		NIST Webbook
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rinpol	658.00		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	657.60		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	666.20		NIST Webbook
rinpol	667.60		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	656.10		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	666.00		NIST Webbook
rinpol	657.00		NIST Webbook
rinpol	656.10		NIST Webbook
rinpol	661.00		NIST Webbook
rinpol	666.00		NIST Webbook
rinpol	667.00		NIST Webbook
rinpol	666.00		NIST Webbook
rinpol	665.80		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	657.60		NIST Webbook
rinpol	657.00		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	656.10		NIST Webbook
rinpol	667.60		NIST Webbook
rinpol	666.20		NIST Webbook
rinpol	667.00		NIST Webbook
rinpol	657.00		NIST Webbook
rinpol	665.60		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	666.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	655.40		NIST Webbook
rinpol	655.10		NIST Webbook
rinpol	665.80		NIST Webbook
rinpol	664.00		NIST Webbook
tb	360.50 ± 1.00	K	NIST Webbook
tb	360.80	K	NIST Webbook

tb	360.79 ± 0.20	K	NIST Webbook
tb	360.73 ± 0.30	K	NIST Webbook
tb	360.71 ± 0.30	K	NIST Webbook
tb	360.85 ± 0.30	K	NIST Webbook
tb	360.50 ± 1.00	K	NIST Webbook
tc	539.72	K	Joback Method
tf	147.46 ± 0.03	K	NIST Webbook
tf	147.42 ± 0.08	K	NIST Webbook
tf	147.46 ± 0.02	K	NIST Webbook
tf	147.42 ± 0.04	K	NIST Webbook
tf	147.41 ± 0.06	K	NIST Webbook
tf	145.41 ± 0.10	K	NIST Webbook
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	245.01	J/mol×K	539.72	Joback Method
dvisc	0.0026515	Pa×s	184.35	Joback Method
dvisc	0.0095853	Pa×s	148.57	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
dvisc	0.0001915	Pa×s	363.28	Joback Method
hvapt	33.60	kJ/mol	349.50	NIST Webbook
hvapt	33.60	kJ/mol	350.50	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39671e+01
Coeff. B	-2.88784e+03
Coeff. C	-5.18100e+01
Temperature range (K), min.	262.92
Temperature range (K), max.	385.45

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=226
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3683225&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
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

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