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

Other names:	(E)-3-Hexene, 3-methyl
	(E)-3-METHYL-3-HEXENE
	3-METHYL-TRANS-3-HEXENE
	3-Methyl-3-hexene, trans
	TRANS-3-METHYL-3-HEXENE
Inchi:	InChI=1S/C7H14/c1-4-6-7(3)5-2/h6H,4-5H2,1-3H3/b7-6+
InchiKey:	FHHSSXNRVNXTBG-VOTSOKGWSA-N
Formula:	C7H14
SMILES:	CCC=C(C)CC
Mol. weight [g/mol]:	98.19
CAS:	3899-36-3

Physical Properties

Property code	Value	Unit	Source
chl	-4642.65 ± 0.88	kJ/mol	NIST Webbook
gf	79.73	kJ/mol	Joback Method
hf	-80.38	kJ/mol	Joback Method
hfus	12.78	kJ/mol	Joback Method
hvap	35.80	kJ/mol	NIST Webbook
hvap	35.80	kJ/mol	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	703.40		NIST Webbook
rinpol	691.20		NIST Webbook
rinpol	703.00		NIST Webbook
rinpol	703.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	689.00		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	686.00		NIST Webbook

rinpol	695.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	703.20		NIST Webbook
rinpol	703.20		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	691.30		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	703.00		NIST Webbook
rinpol	703.00		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	703.00		NIST Webbook
ripol	735.00		NIST Webbook
ripol	731.00		NIST Webbook
tb	366.70 ± 0.30	K	NIST Webbook
tb	366.67 ± 0.20	K	NIST Webbook
tb	366.70	K	NIST Webbook
tc	539.41	K	Joback Method
tf	131.59 ± 0.03	K	NIST Webbook
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.86	J/mol×K	480.80	Joback Method
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	244.29	J/mol×K	539.41	Joback Method
hvapt	34.80	kJ/mol	339.00	NIST Webbook
hvapt	35.30	kJ/mol	333.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41951e+01
Coeff. B	-3.11299e+03
Coeff. C	-4.16350e+01
Temperature range (K), min.	265.47
Temperature range (K), max.	392.05

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.98033e+01
Coeff. B	-7.19630e+03
Coeff. C	-1.13231e+01
Coeff. D	9.64776e-06
Temperature range (K), min.	300.15
Temperature range (K), max.	366.15

Sources

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

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=232

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3899363&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=232

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

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

Legend

chl: Standard liquid enthalpy of combustion

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
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

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