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

Other names: (2Z)-3-Methyl-2-hexene
(Z)-2-Hexene, 3-methyl
(Z)-3-METHYL-2-HEXENE
3-METHYL-CIS-2-HEXENE
CIS-3-METHYL-2-HEXENE
Inchi: InChI=1S/C7H14/c1-4-6-7(3)5-2/h5H,4,6H2,1-3H3/b7-5-
InchiKey: JZMUUSXQSKCZNO-ALCCZGGFSA-N
Formula: C7H14
SMILES: CC=C(C)CCC
Mol. weight [g/mol]: 98.19
CAS: 10574-36-4

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
log10ws	-2.61		Crippen Method
logp	2.753		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	702.00		NIST Webbook
rinpol	694.10		NIST Webbook
rinpol	695.30		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	702.00		NIST Webbook

rinpol	701.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	702.40		NIST Webbook
rinpol	692.60		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	702.50		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	703.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	702.50		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	701.40		NIST Webbook
rinpol	694.40		NIST Webbook
rinpol	695.30		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	694.40		NIST Webbook
rinpol	693.80		NIST Webbook
rinpol	701.70		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	701.40		NIST Webbook
rinpol	710.00		NIST Webbook
ripol	757.00		NIST Webbook
ripol	745.00		NIST Webbook
tb	370.43 ± 0.20	K	NIST Webbook
tb	370.41 ± 0.20	K	NIST Webbook
tb	370.50	K	NIST Webbook
tb	370.43 ± 0.20	K	NIST Webbook
tc	539.41	K	Joback Method
tf	149.61	K	Joback Method
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	34.20	kJ/mol	359.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40937e+01
Coeff. B	-3.06038e+03
Coeff. C	-4.74290e+01
Temperature range (K), min.	269.10
Temperature range (K), max.	395.90

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10574364&Units=SI

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

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=223

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
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