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

Other names:	(Z)-2,2-DIMETHYL-3-HEXENE
	(Z)-2,2-Dimethylhex-3-ene
	2,2-DIMETHYL-CIS-3-HEXENE
	2,2-Dimethyl-3-hexene (cis)
	CIS-2,2-DIMETHYL-3-HEXENE
Inchi:	InChI=1S/C8H16/c1-5-6-7-8(2,3)4/h6-7H,5H2,1-4H3/b7-6-
InchiKey:	JPLZSSHKQZJYTJ-SREVYHEPSA-N
Formula:	C8H16
SMILES:	CCC=CC(C)(C)C
Mol. weight [g/mol]:	112.21
CAS:	690-92-6

Physical Properties

Property code	Value	Unit	Source
chl	-5288.45 ± 0.71	kJ/mol	NIST Webbook
chl	-5308.30 ± 2.50	kJ/mol	NIST Webbook
chl	-5298.40 ± 1.50	kJ/mol	NIST Webbook
gf	99.54	kJ/mol	Joback Method
hf	-96.60	kJ/mol	NIST Webbook
hfl	-136.40 ± 1.50	kJ/mol	NIST Webbook
hfus	9.26	kJ/mol	Joback Method
hvap	37.10	kJ/mol	NIST Webbook
hvap	37.20	kJ/mol	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
rinpol	719.00		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	715.20		NIST Webbook
rinpol	716.10		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	714.00		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	718.70		NIST Webbook
rinpol	714.50		NIST Webbook

rinpol	722.00		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	723.60		NIST Webbook
rinpol	718.70		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	724.70		NIST Webbook
rinpol	723.60		NIST Webbook
rinpol	723.20		NIST Webbook
rinpol	717.00		NIST Webbook
tb	379.00 ± 0.50	K	NIST Webbook
tb	378.70	K	NIST Webbook
tb	378.95 ± 0.60	K	NIST Webbook
tc	566.77	K	Joback Method
tf	135.80 ± 0.03	K	NIST Webbook
tf	135.77 ± 0.05	K	NIST Webbook
tf	135.80 ± 0.03	K	NIST Webbook
tf	135.77 ± 0.06	K	NIST Webbook
tf	135.76 ± 0.07	K	NIST Webbook
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.13	J/mol×K	383.37	Joback Method
cpg	233.64	J/mol×K	413.94	Joback Method
cpg	247.38	J/mol×K	444.50	Joback Method
cpg	260.39	J/mol×K	475.07	Joback Method
cpg	272.68	J/mol×K	505.64	Joback Method
cpg	284.31	J/mol×K	536.21	Joback Method
cpg	295.30	J/mol×K	566.77	Joback Method
dvisc	0.0034054	Pa×s	211.61	Joback Method
dvisc	0.0110015	Pa×s	177.26	Joback Method
dvisc	0.0014626	Pa×s	245.96	Joback Method
dvisc	0.0007728	Pa×s	280.31	Joback Method
dvisc	0.0004693	Pa×s	314.67	Joback Method
dvisc	0.0003144	Pa×s	349.02	Joback Method
dvisc	0.0002263	Pa×s	383.37	Joback Method
hvapt	35.30	kJ/mol	349.50	NIST Webbook

hvapt	36.10	kJ/mol	342.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37491e+01
Coeff. B	-2.93879e+03
Coeff. C	-5.68450e+01
Temperature range (K), min.	275.16
Temperature range (K), max.	405.14

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.78581e+01
Coeff. B	-7.67064e+03
Coeff. C	-1.25413e+01
Coeff. D	1.02697e-05
Temperature range (K), min.	305.15
Temperature range (K), max.	378.15

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C690926&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=310

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=310

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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