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

Other names:	(E)-2,2-DIMETHYL-3-HEXENE
	(E)-2,2-Dimethylhex-3-ene
	2,2-DIMETHYL-TRANS-3-HEXENE
	TRANS-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-VOTSOKGWSA-N
Formula:	C8H16
SMILES:	CCC=CC(C)(C)C
Mol. weight [g/mol]:	112.21
CAS:	690-93-7

Physical Properties

Property code	Value	Unit	Source
chl	-5289.70 ± 1.20	kJ/mol	NIST Webbook
chl	-5267.00 ± 1.40	kJ/mol	NIST Webbook
chl	-5276.90 ± 2.00	kJ/mol	NIST Webbook
gf	99.54	kJ/mol	Joback Method
hf	-118.00	kJ/mol	NIST Webbook
hfl	-157.80 ± 2.00	kJ/mol	NIST Webbook
hfus	9.26	kJ/mol	Joback Method
hvap	37.20	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	710.00		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	710.50		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	709.00		NIST Webbook
rinpol	693.20		NIST Webbook
rinpol	692.00		NIST Webbook
tb	374.65 ± 1.50	K	NIST Webbook

tb	374.05 ± 0.60	K	NIST Webbook
tb	374.18 ± 0.30	K	NIST Webbook
tb	374.00	K	NIST Webbook
tb	374.18 ± 0.30	K	NIST Webbook
tc	566.77	K	Joback Method
tf	177.26	K	Joback Method
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	36.10	kJ/mol	342.50	NIST Webbook
hvapt	36.30	kJ/mol	338.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36354e+01
Coeff. B	-2.80501e+03
Coeff. C	-6.29230e+01
Temperature range (K), min.	273.07
Temperature range (K), max.	399.90

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.02382e+02
Coeff. B	-7.85307e+03
Coeff. C	-1.32200e+01
Coeff. D	1.10860e-05
Temperature range (K), min.	302.15
Temperature range (K), max.	374.15

Sources

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=311
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C690937&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=311
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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