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

Other names:	(Z)-3-METHYL-2-PENTENE
	(Z)-3-methylpent-2-ene
	(Z)-CH3CH=C(CH3)C2H5
	3-METHYL-CIS-2-PENTENE
	3-Methyl-2-pentene, cis
	CIS-3-METHYL-2-PENTENE
Inchi:	InChI=1S/C6H12/c1-4-6(3)5-2/h4H,5H2,1-3H3/b6-4-
InchiKey:	BEQGRRJLJLVQAQ-XQRVVYSFSA-N
Formula:	C6H12
SMILES:	CC=C(C)CC
Mol. weight [g/mol]:	84.16
CAS:	922-62-3

Physical Properties

Property code	Value	Unit	Source
af	0.2690		KDB
gf	73.27	kJ/mol	KDB
hcg	3981.70	kJ/mol	KDB
hcn	3717.610	kJ/mol	KDB
hf	-61.88 ± 0.88	kJ/mol	NIST Webbook
hf	-62.22	kJ/mol	KDB
hfl	-94.06 ± 0.84	kJ/mol	NIST Webbook
hfus	10.19	kJ/mol	Joback Method
hvap	32.10	kJ/mol	NIST Webbook
hvap	32.10	kJ/mol	NIST Webbook
hvap	31.30	kJ/mol	NIST Webbook
ie	8.58	eV	NIST Webbook
ie	8.58	eV	NIST Webbook
log10ws	-2.19		Crippen Method
logp	2.363		Crippen Method
mcvol	91.100	ml/mol	McGowan Method
pc	3280.00	kPa	KDB
rinpol	601.80		NIST Webbook
rinpol	610.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	614.80		NIST Webbook
rinpol	615.00		NIST Webbook

rinpol	615.20	NIST Webbook
rinpol	615.50	NIST Webbook
rinpol	615.70	NIST Webbook
rinpol	616.00	NIST Webbook
rinpol	610.00	NIST Webbook
rinpol	610.00	NIST Webbook
rinpol	610.60	NIST Webbook
rinpol	611.30	NIST Webbook
rinpol	612.00	NIST Webbook
rinpol	612.70	NIST Webbook
rinpol	613.40	NIST Webbook
rinpol	611.00	NIST Webbook
rinpol	611.30	NIST Webbook
rinpol	611.00	NIST Webbook
rinpol	611.00	NIST Webbook
rinpol	610.90	NIST Webbook
rinpol	610.90	NIST Webbook
rinpol	617.00	NIST Webbook
rinpol	603.00	NIST Webbook
rinpol	612.10	NIST Webbook
rinpol	602.40	NIST Webbook
rinpol	603.00	NIST Webbook
rinpol	603.00	NIST Webbook
rinpol	601.55	NIST Webbook
rinpol	602.00	NIST Webbook
rinpol	602.00	NIST Webbook
rinpol	603.00	NIST Webbook
rinpol	605.00	NIST Webbook
rinpol	605.00	NIST Webbook
rinpol	613.00	NIST Webbook
rinpol	612.50	NIST Webbook
rinpol	613.00	NIST Webbook
rinpol	615.00	NIST Webbook
rinpol	610.00	NIST Webbook
rinpol	610.54	NIST Webbook
rinpol	611.00	NIST Webbook
rinpol	611.00	NIST Webbook
rinpol	608.00	NIST Webbook
rinpol	602.60	NIST Webbook
rinpol	613.00	NIST Webbook
rinpol	619.00	NIST Webbook
rinpol	607.00	NIST Webbook
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rinpol	610.00		NIST Webbook
rinpol	613.00		NIST Webbook
rinpol	610.20		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	606.00		NIST Webbook
rinpol	610.00		NIST Webbook
ripol	672.00		NIST Webbook
ripol	660.00		NIST Webbook
tb	339.10 ± 1.00	K	NIST Webbook
tb	339.10 ± 2.00	K	NIST Webbook
tb	338.55 ± 3.00	K	NIST Webbook
tb	340.90	K	KDB
tb	340.90	K	NIST Webbook
tb	340.86 ± 0.20	K	NIST Webbook
tb	343.67 ± 0.50	K	NIST Webbook
tb	340.84 ± 0.30	K	NIST Webbook
tb	340.85 ± 0.50	K	NIST Webbook
tb	340.85 ± 0.30	K	NIST Webbook
tb	341.15 ± 1.00	K	NIST Webbook
tb	340.95 ± 0.50	K	NIST Webbook
tb	340.65 ± 0.70	K	NIST Webbook
tb	340.95 ± 0.20	K	NIST Webbook
tb	340.95 ± 0.60	K	NIST Webbook
tb	338.55 ± 1.00	K	NIST Webbook
tb	341.15 ± 1.00	K	NIST Webbook
tb	338.80 ± 2.00	K	NIST Webbook
tc	518.00	K	KDB
tf	138.30	K	KDB
tf	138.31 ± 0.05	K	NIST Webbook
tf	137.40 ± 0.60	K	NIST Webbook
tf	137.75 ± 0.20	K	NIST Webbook
vc	0.351	m3/kmol	KDB
zc	0.2673100		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.07	J/mol×K	340.72	Joback Method
cpg	155.60	J/mol×K	370.05	Joback Method
cpg	165.66	J/mol×K	399.37	Joback Method
cpg	175.29	J/mol×K	428.70	Joback Method
cpg	184.49	J/mol×K	458.03	Joback Method
cpg	193.27	J/mol×K	487.36	Joback Method
cpg	201.67	J/mol×K	516.68	Joback Method
hvapt	28.83	kJ/mol	340.90	KDB
hvapt	32.20	kJ/mol	312.00	NIST Webbook
rfi	1.39876		298.15	KDB
rhol	694.00	kg/m3	293.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42373e+01
Coeff. B	-2.95465e+03
Coeff. C	-3.36810e+01
Temperature range (K), min.	245.49
Temperature range (K), max.	364.70

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.85178e+01
Coeff. B	-5.87552e+03
Coeff. C	-8.14977e+00
Coeff. D	7.21031e-06
Temperature range (K), min.	138.31
Temperature range (K), max.	515.00

Sources

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=205
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=205
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C922623&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
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
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
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

zc: Critical Compressibility