2-Pentene, 2-methyl-

Other names:	(CH3)2C=CHC2H5
	1,1-dimethyl-1-butene
	2,4-dimethyl-2-butene
	2-Methyl-2-pentene
	2-Methyl-pentene-2
	2-Methylpent-2-ene
	2-ethyl-1,1-dimethylethylene
	2-pentene, 2-methyl
	4-METHYL-3-PENTENE
Inchi:	InChI=1S/C6H12/c1-4-5-6(2)3/h5H,4H2,1-3H3
InchiKey:	JMMZCWZIJXAGKW-UHFFFAOYSA-N
Formula:	C6H12
SMILES:	CCC=C(C)C
Mol. weight [g/mol]:	84.16
CAS:	625-27-4

Physical Properties

Property code	Value	Unit	Source
af	0.2290		KDB
affp	812.00	kJ/mol	NIST Webbook
basg	783.10	kJ/mol	NIST Webbook
gf	71.26	kJ/mol	KDB
hcg	3977.56	kJ/mol	KDB
hcn	3713.467	kJ/mol	KDB
hf	-66.53	kJ/mol	KDB
hfus	10.19	kJ/mol	Joback Method
hvap	31.60	kJ/mol	NIST Webbook
hvap	31.60	kJ/mol	NIST Webbook
hvap	31.60	kJ/mol	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
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=1)		KDB
pc	3280.00	kPa	KDB
rinpol	607.00		NIST Webbook

rinpol	604.60	NIST Webbook
rinpol	598.00	NIST Webbook
rinpol	597.70	NIST Webbook
rinpol	607.30	NIST Webbook
rinpol	597.70	NIST Webbook
rinpol	598.00	NIST Webbook
rinpol	605.00	NIST Webbook
rinpol	605.00	NIST Webbook
rinpol	606.00	NIST Webbook
rinpol	606.00	NIST Webbook
rinpol	606.00	NIST Webbook
rinpol	606.20	NIST Webbook
rinpol	606.00	NIST Webbook
rinpol	598.10	NIST Webbook
rinpol	597.90	NIST Webbook
rinpol	607.00	NIST Webbook
rinpol	607.00	NIST Webbook
rinpol	606.00	NIST Webbook
rinpol	606.00	NIST Webbook
rinpol	606.00	NIST Webbook
rinpol	606.00	NIST Webbook
rinpol	606.00	NIST Webbook
rinpol	606.00	NIST Webbook
rinpol	611.50	NIST Webbook
rinpol	611.30	NIST Webbook
rinpol	611.10	NIST Webbook
rinpol	610.90	NIST Webbook
rinpol	610.70	NIST Webbook
rinpol	610.50	NIST Webbook
rinpol	606.00	NIST Webbook
rinpol	600.00	NIST Webbook
rinpol	606.00	NIST Webbook
rinpol	606.40	NIST Webbook
rinpol	606.80	NIST Webbook
rinpol	607.20	NIST Webbook
rinpol	607.60	NIST Webbook
rinpol	608.00	NIST Webbook
rinpol	608.50	NIST Webbook
rinpol	606.30	NIST Webbook
rinpol	606.60	NIST Webbook
rinpol	606.50	NIST Webbook
rinpol	606.40	NIST Webbook
rinpol	610.90	NIST Webbook
rinpol	606.40	NIST Webbook

rinpol	598.00	NIST Webbook
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rinpol	597.30	NIST Webbook
rinpol	595.00	NIST Webbook
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rinpol	598.00	NIST Webbook
rinpol	597.56	NIST Webbook
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rinpol	600.00		NIST Webbook
rinpol	587.18		NIST Webbook
rinpol	599.00		NIST Webbook
ripol	642.00		NIST Webbook
ripol	654.00		NIST Webbook
tb	273.15 ± 0.40	K	NIST Webbook
tb	340.05 ± 0.50	K	NIST Webbook
tb	340.50	K	KDB
tb	340.50	K	NIST Webbook
tb	340.41 ± 0.20	K	NIST Webbook
tb	339.70 ± 1.00	K	NIST Webbook
tb	338.15 ± 2.00	K	NIST Webbook
tb	339.15 ± 2.00	K	NIST Webbook
tb	340.51 ± 0.20	K	NIST Webbook
tb	340.44 ± 0.20	K	NIST Webbook
tb	340.45 ± 0.30	K	NIST Webbook
tb	340.45 ± 0.30	K	NIST Webbook
tb	340.41 ± 0.30	K	NIST Webbook
tb	349.45 ± 0.30	K	NIST Webbook
tb	340.41 ± 0.30	K	NIST Webbook
tb	340.40 ± 0.30	K	NIST Webbook
tb	340.42 ± 0.30	K	NIST Webbook
tb	340.40 ± 0.30	K	NIST Webbook
tb	340.50 ± 0.50	K	NIST Webbook
tb	339.15 ± 2.00	K	NIST Webbook
tb	340.35 ± 0.50	K	NIST Webbook
tb	340.35 ± 0.60	K	NIST Webbook
tb	340.25 ± 0.50	K	NIST Webbook
tb	339.65 ± 3.00	K	NIST Webbook
tb	340.10 ± 1.00	K	NIST Webbook
tb	340.35 ± 0.60	K	NIST Webbook
tb	340.50 ± 0.60	K	NIST Webbook
tc	518.00	K	KDB
tc	509.30	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	138.04 ± 0.30	K	NIST Webbook
tf	137.99 ± 0.40	K	NIST Webbook
tf	138.10	K	KDB
tf	138.09 ± 0.30	K	NIST Webbook

tf	138.04 ± 0.40	K	NIST Webbook
tf	138.40 ± 0.50	K	NIST Webbook
tf	138.50 ± 0.30	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	193.27	J/mol×K	487.36	Joback Method
cpg	184.49	J/mol×K	458.03	Joback Method
cpg	175.29	J/mol×K	428.70	Joback Method
cpg	165.66	J/mol×K	399.37	Joback Method
cpg	155.60	J/mol×K	370.05	Joback Method
cpg	201.67	J/mol×K	516.68	Joback Method
hvapt	32.40	kJ/mol	311.50	NIST Webbook
hvapt	29.00	kJ/mol	340.50	KDB
rfi	1.40030		293.15	A novel static analytical apparatus for phase equilibrium measurements
rfi	1.39739		298.15	KDB
rhol	691.00	kg/m3	289.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40723e+01
Coeff. B	-2.86838e+03
Coeff. C	-3.70430e+01
Temperature range (K), min.	245.13
Temperature range (K), max.	364.46

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.70586e+01
Coeff. B	-5.92015e+03
Coeff. C	-7.83366e+00
Coeff. D	5.36185e-06
Temperature range (K), min.	138.07
Temperature range (K), max.	514.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=204
Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
KDB:	https://www.cheric.org/files/research/kdb/mol/mol204.mol
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C625274&Units=SI
A novel static analytical apparatus for phase equilibrium measurements:	https://www.doi.org/10.1016/j.fluid.2012.11.008

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
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
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
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

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