1-Pentene, 4-methyl-

Other names:	(CH3)2CHCH2CH=CH2
	4-Methyl-1-pentene
	4-Methylpentene-(1)
	4-methylpent-1-ene
	ISOBUTYLETHENE
Inchi:	InChI=1S/C6H12/c1-4-5-6(2)3/h4,6H,1,5H2,2-3H3
InchiKey:	WSSSPWUEQFSQQG-UHFFFAOYSA-N
Formula:	C6H12
SMILES:	C=CCC(C)C
Mol. weight [g/mol]:	84.16
CAS:	691-37-2

Physical Properties

Property code	Value	Unit	Source
af	0.2620		KDB
chl	-3997.82 ± 0.54	kJ/mol	NIST Webbook
gf	85.04	kJ/mol	Joback Method
hcg	3996.10	kJ/mol	KDB
hcn	3732.002	kJ/mol	KDB
hf	-49.44 ± 0.67	kJ/mol	NIST Webbook
hfl	-78.22 ± 0.64	kJ/mol	NIST Webbook
hfus	6.49	kJ/mol	Joback Method
hvap	28.70	kJ/mol	NIST Webbook
hvap	28.60 ± 0.20	kJ/mol	NIST Webbook
hvap	28.70	kJ/mol	NIST Webbook
hvap	28.70	kJ/mol	NIST Webbook
hvap	28.80 ± 0.20	kJ/mol	NIST Webbook
ie	9.45 ± 0.02	eV	NIST Webbook
ie	9.45 ± 0.00	eV	NIST Webbook
ie	9.44	eV	NIST Webbook
ie	9.45 ± 0.01	eV	NIST Webbook
log10ws	-3.24		Aqueous Solubility Prediction Method
logp	2.219		Crippen Method
mcvol	91.100	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=1)		KDB

pc	3290.00 ± 150.00	kPa	NIST Webbook
pc	3290.00	kPa	KDB
rhoc	238.17 ± 10.10	kg/m3	NIST Webbook
rinpol	549.00		NIST Webbook
rinpol	560.20		NIST Webbook
rinpol	560.40		NIST Webbook
rinpol	560.70		NIST Webbook
rinpol	555.70		NIST Webbook
rinpol	556.40		NIST Webbook
rinpol	557.00		NIST Webbook
rinpol	557.60		NIST Webbook
rinpol	558.40		NIST Webbook
rinpol	559.10		NIST Webbook
rinpol	562.00		NIST Webbook
rinpol	560.90		NIST Webbook
rinpol	559.40		NIST Webbook
rinpol	558.00		NIST Webbook
rinpol	556.50		NIST Webbook
rinpol	555.10		NIST Webbook
rinpol	551.00		NIST Webbook
rinpol	549.00		NIST Webbook
rinpol	556.00		NIST Webbook
rinpol	549.00		NIST Webbook
rinpol	549.00		NIST Webbook
rinpol	550.00		NIST Webbook
rinpol	550.00		NIST Webbook
rinpol	549.00		NIST Webbook
rinpol	550.00		NIST Webbook
rinpol	547.94		NIST Webbook
rinpol	559.00		NIST Webbook
rinpol	551.00		NIST Webbook
rinpol	559.00		NIST Webbook
rinpol	560.00		NIST Webbook
rinpol	550.00		NIST Webbook
rinpol	551.00		NIST Webbook
rinpol	552.00		NIST Webbook
rinpol	557.00		NIST Webbook
rinpol	554.00		NIST Webbook
rinpol	561.70		NIST Webbook
rinpol	560.00		NIST Webbook
rinpol	554.60		NIST Webbook
rinpol	547.00		NIST Webbook
rinpol	549.00		NIST Webbook
rinpol	560.00		NIST Webbook

rinpol	549.00	NIST Webbook
rinpol	549.00	NIST Webbook
rinpol	568.00	NIST Webbook
rinpol	553.00	NIST Webbook
rinpol	558.00	NIST Webbook
rinpol	548.00	NIST Webbook
rinpol	546.00	NIST Webbook
rinpol	554.00	NIST Webbook
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rinpol	554.00	NIST Webbook
rinpol	554.60	NIST Webbook
rinpol	559.80	NIST Webbook
rinpol	559.60	NIST Webbook
rinpol	556.00	NIST Webbook
rinpol	556.00	NIST Webbook
rinpol	550.80	NIST Webbook
rinpol	549.70	NIST Webbook
rinpol	556.00	NIST Webbook
rinpol	559.20	NIST Webbook
rinpol	558.70	NIST Webbook
rinpol	550.40	NIST Webbook
rinpol	557.10	NIST Webbook
rinpol	556.70	NIST Webbook
rinpol	557.10	NIST Webbook
rinpol	556.70	NIST Webbook
rinpol	554.00	NIST Webbook
rinpol	548.00	NIST Webbook
rinpol	548.10	NIST Webbook
rinpol	556.20	NIST Webbook
rinpol	549.40	NIST Webbook
rinpol	556.80	NIST Webbook

ripol	595.00		NIST Webbook
ripol	589.00		NIST Webbook
ripol	595.00		NIST Webbook
tb	326.90 ± 0.60	K	NIST Webbook
tb	326.65 ± 2.00	K	NIST Webbook
tb	326.90 ± 0.60	K	NIST Webbook
tb	327.20 ± 0.40	K	NIST Webbook
tb	326.70 ± 3.00	K	NIST Webbook
tb	327.00	K	KDB
tb	327.10	K	NIST Webbook
tb	326.95 ± 0.50	K	NIST Webbook
tb	327.05 ± 0.50	K	NIST Webbook
tb	327.04 ± 0.20	K	NIST Webbook
tb	327.15 ± 0.50	K	NIST Webbook
tb	326.98 ± 0.30	K	NIST Webbook
tb	327.10 ± 0.30	K	NIST Webbook
tb	327.10 ± 0.30	K	NIST Webbook
tb	327.03 ± 0.20	K	NIST Webbook
tb	326.95 ± 0.50	K	NIST Webbook
tb	327.10 ± 0.20	K	NIST Webbook
tb	327.15 ± 0.40	K	NIST Webbook
tb	327.10 ± 0.20	K	NIST Webbook
tb	326.90 ± 0.50	K	NIST Webbook
tb	326.95 ± 0.40	K	NIST Webbook
tb	326.91 ± 0.20	K	NIST Webbook
tc	493.10	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tc	494.80	K	KDB
tc	495.00 ± 2.00	K	NIST Webbook
tf	118.16 ± 0.20	K	NIST Webbook
tf	119.31 ± 0.30	K	NIST Webbook
tf	119.14 ± 0.50	K	NIST Webbook
tf	119.20 ± 0.15	K	NIST Webbook
tf	168.10 ± 0.40	K	NIST Webbook
tf	119.62	K	Aqueous Solubility Prediction Method
tf	120.00	K	KDB
tf	119.11 ± 0.30	K	NIST Webbook
tf	119.10 ± 0.40	K	NIST Webbook
vc	0.346	m3/kmol	KDB
zc	0.2770980		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.52	J/mol×K	332.92	Joback Method
cpg	155.75	J/mol×K	361.38	Joback Method
cpg	165.59	J/mol×K	389.85	Joback Method
cpg	175.03	J/mol×K	418.31	Joback Method
cpg	184.10	J/mol×K	446.78	Joback Method
cpg	192.81	J/mol×K	475.24	Joback Method
cpg	201.16	J/mol×K	503.71	Joback Method
dvisc	0.0002133	Pa×s	332.92	Joback Method
dvisc	0.0022681	Pa×s	172.67	Joback Method
dvisc	0.0010513	Pa×s	204.72	Joback Method
dvisc	0.0069474	Pa×s	140.62	Joback Method
dvisc	0.0003915	Pa×s	268.82	Joback Method
dvisc	0.0002798	Pa×s	300.87	Joback Method
dvisc	0.0006001	Pa×s	236.77	Joback Method
hfust	4.93	kJ/mol	118.90	NIST Webbook
hvapt	27.07	kJ/mol	327.00	KDB
hvapt	27.40 ± 0.30	kJ/mol	335.00	NIST Webbook
hvapt	26.20 ± 0.40	kJ/mol	335.00	NIST Webbook
hvapt	24.90 ± 0.50	kJ/mol	335.00	NIST Webbook
hvapt	30.10	kJ/mol	299.00	NIST Webbook
rfi	1.37974		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41104e+01
Coeff. B	-2.79799e+03
Coeff. C	-3.22380e+01
Temperature range (K), min.	234.66
Temperature range (K), max.	350.23

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.91163e+01
Coeff. B	-5.94790e+03
Coeff. C	-9.91273e+00
Coeff. D	1.01493e-05
Temperature range (K), min.	119.51
Temperature range (K), max.	496.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C691372&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=203
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB:	https://www.cheric.org/files/research/kdb/mol/mol203.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
hfust:	Enthalpy of fusion at a given temperature
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
rhoc:	Critical density
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
zc:	Critical Compressibility