1-Pentene, 4,4-dimethyl-

Other names:	(CH3)3CCH2CH=CH2
	2,2-DIMETHYL-4-PENTENE
	4,4-Dimethyl-1-pentene
	4,4-dimethylpent-1-ene
	neo-amylethylene
Inchi:	InChI=1S/C7H14/c1-5-6-7(2,3)4/h5H,1,6H2,2-4H3
InchiKey:	KLCNJIQZXOQYTE-UHFFFAOYSA-N
Formula:	C7H14
SMILES:	C=CCC(C)(C)C
Mol. weight [g/mol]:	98.19
CAS:	762-62-9

Physical Properties

Property code	Value	Unit	Source
chl	-4644.80 ± 1.70	kJ/mol	NIST Webbook
gf	98.74	kJ/mol	Joback Method
hf	-71.13	kJ/mol	Joback Method
hfus	5.19	kJ/mol	Joback Method
hvap	31.20	kJ/mol	NIST Webbook
hvap	31.20	kJ/mol	NIST Webbook
ie	9.60	eV	NIST Webbook
ie	9.40 ± 0.00	eV	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.609		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	605.00		NIST Webbook
rinpol	605.00		NIST Webbook
rinpol	605.00		NIST Webbook
rinpol	606.00		NIST Webbook
rinpol	605.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	605.00		NIST Webbook
rinpol	607.00		NIST Webbook
rinpol	609.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	610.00		NIST Webbook

rinpol	610.00		NIST Webbook
rinpol	608.00		NIST Webbook
rinpol	603.40		NIST Webbook
rinpol	608.00		NIST Webbook
rinpol	607.00		NIST Webbook
rinpol	606.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	607.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	609.00		NIST Webbook
rinpol	608.00		NIST Webbook
rinpol	608.00		NIST Webbook
rinpol	610.40		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	606.00		NIST Webbook
rinpol	609.00		NIST Webbook
rinpol	603.40		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	606.60		NIST Webbook
rinpol	604.90		NIST Webbook
rinpol	615.90		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	602.30		NIST Webbook
rinpol	614.50		NIST Webbook
rinpol	610.40		NIST Webbook
tb	345.25 ± 0.50	K	NIST Webbook
tb	345.59 ± 0.20	K	NIST Webbook
tb	345.30 ± 0.30	K	NIST Webbook
tb	344.40 ± 4.00	K	NIST Webbook
tb	345.25 ± 0.40	K	NIST Webbook
tb	344.40 ± 0.50	K	NIST Webbook
tb	344.95 ± 0.60	K	NIST Webbook
tb	345.70	K	NIST Webbook
tb	345.58 ± 0.20	K	NIST Webbook
tb	345.65 ± 0.50	K	NIST Webbook
tb	345.10 ± 3.00	K	NIST Webbook
tb	345.65 ± 0.30	K	NIST Webbook
tb	345.35 ± 0.50	K	NIST Webbook
tb	345.66 ± 0.30	K	NIST Webbook

tb	345.65 ± 0.20	K	NIST Webbook
tb	345.50 ± 1.00	K	NIST Webbook
tc	516.00	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	136.45 ± 0.50	K	NIST Webbook
tf	136.45 ± 0.30	K	NIST Webbook
tf	136.50 ± 0.50	K	NIST Webbook
tf	136.55 ± 0.03	K	NIST Webbook
tf	136.51 ± 0.06	K	NIST Webbook
tf	135.53 ± 0.50	K	NIST Webbook
tf	136.50 ± 0.40	K	NIST Webbook
tf	136.47 ± 0.20	K	NIST Webbook
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.87	J/mol×K	353.01	Joback Method
cpg	193.78	J/mol×K	382.73	Joback Method
cpg	206.04	J/mol×K	412.45	Joback Method
cpg	217.68	J/mol×K	442.17	Joback Method
cpg	228.72	J/mol×K	471.89	Joback Method
cpg	239.19	J/mol×K	501.61	Joback Method
cpg	249.12	J/mol×K	531.33	Joback Method
dvisc	0.0032853	Pa×s	199.93	Joback Method
dvisc	0.0092538	Pa×s	169.31	Joback Method
dvisc	0.0015356	Pa×s	230.54	Joback Method
dvisc	0.0008579	Pa×s	261.16	Joback Method
dvisc	0.0005415	Pa×s	291.78	Joback Method
dvisc	0.0003731	Pa×s	322.39	Joback Method
dvisc	0.0002742	Pa×s	353.01	Joback Method
hvapt	31.00	kJ/mol	323.00	NIST Webbook
hvapt	31.00	kJ/mol	318.00	NIST Webbook

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38019e+01
Coeff. B	-2.74766e+03
Coeff. C	-4.64750e+01
Temperature range (K), min.	249.79
Temperature range (K), max.	370.09

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.95616e+01
Coeff. B	-6.26895e+03
Coeff. C	-9.90657e+00
Coeff. D	9.21539e-06
Temperature range (K), min.	290.15
Temperature range (K), max.	345.15

Sources

Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=239
KDB:	https://www.cheric.org/files/research/kdb/mol/mol239.mol
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C762629&Units=SI

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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume