2-Pentene, 4,4-dimethyl-, (E)-

Other names:	(E)-(CH3)3CCH=CHCH3
	(E)-4,4-DIMETHYL-2-PENETENE
	(E)-4,4-Dimethyl-2-pentene
	(E)-4,4-dimethylpent-2-ene
	4,4-DIMETHYL-TRANS-2-PENTENE
	4,4-Dimethyl-(E)-2-pentene
	4,4-Dimethyl-2-pentene, trans
	TRANS-4,4-DIMETHYL-2-PENTENE
Inchi:	InChI=1S/C7H14/c1-5-6-7(2,3)4/h5-6H,1-4H3/b6-5+
InchiKey:	BIDIHFPLDRSAMB-AATRIKPKSA-N
Formula:	C7H14
SMILES:	CC=CC(C)(C)C
Mol. weight [g/mol]:	98.19
CAS:	690-08-4

Physical Properties

Property code	Value	Unit	Source
chl	-4633.61 ± 0.84	kJ/mol	NIST Webbook
gf	91.12	kJ/mol	Joback Method
hf	-79.34	kJ/mol	Joback Method
hfus	6.67	kJ/mol	Joback Method
hvap	32.80	kJ/mol	NIST Webbook
hvap	32.80	kJ/mol	NIST Webbook
ie	8.91 ± 0.01	eV	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.609		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	622.00		NIST Webbook
rinpol	625.90		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	623.10		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	620.00		NIST Webbook
rinpol	625.50		NIST Webbook
rinpol	614.80		NIST Webbook

rinpol	622.00		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	621.30		NIST Webbook
rinpol	621.20		NIST Webbook
rinpol	614.70		NIST Webbook
rinpol	614.70		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	614.50		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	623.10		NIST Webbook
rinpol	625.90		NIST Webbook
rinpol	614.80		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	616.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	622.00		NIST Webbook
tb	349.90 ± 0.20	K	NIST Webbook
tb	349.20 ± 0.50	K	NIST Webbook
tb	349.20 ± 1.00	K	NIST Webbook
tb	350.00 ± 0.50	K	NIST Webbook
tb	349.90	K	NIST Webbook
tb	349.88 ± 0.30	K	NIST Webbook
tb	349.89 ± 0.30	K	NIST Webbook
tb	349.88 ± 0.30	K	NIST Webbook
tc	544.64	K	Joback Method
tf	157.82 ± 0.40	K	NIST Webbook
tf	157.91 ± 0.02	K	NIST Webbook
tf	157.88 ± 0.06	K	NIST Webbook
tf	157.84 ± 0.20	K	NIST Webbook
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.74	J/mol×K	513.95	Joback Method
cpg	250.78	J/mol×K	544.64	Joback Method
cpg	180.91	J/mol×K	360.49	Joback Method
cpg	194.27	J/mol×K	391.18	Joback Method
cpg	206.90	J/mol×K	421.87	Joback Method
cpg	218.84	J/mol×K	452.57	Joback Method
cpg	230.11	J/mol×K	483.26	Joback Method
dvisc	0.0002301	Pa×s	360.49	Joback Method
dvisc	0.0003185	Pa×s	328.07	Joback Method
dvisc	0.0108776	Pa×s	165.99	Joback Method
dvisc	0.0033838	Pa×s	198.41	Joback Method
dvisc	0.0014612	Pa×s	230.82	Joback Method
dvisc	0.0007760	Pa×s	263.24	Joback Method
dvisc	0.0004734	Pa×s	295.66	Joback Method
hvapt	33.00	kJ/mol	319.50	NIST Webbook
hvapt	32.80	kJ/mol	323.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36860e+01
Coeff. B	-2.69730e+03
Coeff. C	-5.22350e+01
Temperature range (K), min.	253.55
Temperature range (K), max.	374.32

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.75118e+01
Coeff. B	-6.38190e+03
Coeff. C	-9.51062e+00

Coeff. D	8.70909e-06
Temperature range (K), min.	288.15
Temperature range (K), max.	350.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C690084&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=246
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=246
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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