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

Other names:	(Z)-(CH3)3CCH=CHCH3
	(Z)-4,4-DIMETHYL-2-PENTENE
	(Z)-4,4-dimethylpent-2-ene
	4,4-DIMETHYL-CIS-2-PENTENE
	CIS-4,4-DIMETHYL-2-PENTENE
Inchi:	InChI=1S/C7H14/c1-5-6-7(2,3)4/h5-6H,1-4H3/b6-5-
InchiKey:	BIDIHFPLDRSAMB-WAYWQWQTSA-N
Formula:	C7H14
SMILES:	CC=CC(C)(C)C
Mol. weight [g/mol]:	98.19
CAS:	762-63-0

Physical Properties

Property code	Value	Unit	Source
chl	-4650.10 ± 1.20	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	32.60	kJ/mol	NIST Webbook
hvap	32.60	kJ/mol	NIST Webbook
ie	8.92 ± 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	635.80		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	645.10		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	633.30		NIST Webbook
rinpol	644.00		NIST Webbook
rinpol	646.00		NIST Webbook
rinpol	648.00		NIST Webbook
rinpol	645.10		NIST Webbook
rinpol	646.90		NIST Webbook
rinpol	635.80		NIST Webbook

rinpol	637.80		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	638.10		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	637.00		NIST Webbook
rinpol	633.00		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	642.80		NIST Webbook
rinpol	644.90		NIST Webbook
rinpol	634.30		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	645.00		NIST Webbook
rinpol	644.90		NIST Webbook
rinpol	642.80		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	634.30		NIST Webbook
tb	360.49	K	Joback Method
tc	544.64	K	Joback Method
tf	165.99	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	240.74	J/mol×K	513.95	Joback Method
cpg	250.78	J/mol×K	544.64	Joback Method

dvisc	0.0033838	Pa×s	198.41	Joback Method
dvisc	0.0108776	Pa×s	165.99	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
dvisc	0.0003185	Pa×s	328.07	Joback Method
dvisc	0.0002301	Pa×s	360.49	Joback Method
hvapt	32.20	kJ/mol	329.00	NIST Webbook
hvapt	32.60	kJ/mol	322.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38487e+01
Coeff. B	-2.82013e+03
Coeff. C	-4.74730e+01
Temperature range (K), min.	255.43
Temperature range (K), max.	377.81

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.29744e+01
Coeff. B	-6.56350e+03
Coeff. C	-1.03910e+01
Coeff. D	9.45622e-06
Temperature range (K), min.	290.15
Temperature range (K), max.	353.15

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C762630&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=245

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=245

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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