2-Pentene, 3,4-dimethyl-, (E)-

Other names:	(2E)-3,4-Dimethyl-2-pentene
	(E)-(CH3)2C=CHCH(CH3)2
	(E)-3,4-DIMETHYL-2-PENTENE
	3,4-DIMETHYL-TRANS-2-PENTENE
	3,4-Dimethyl-2-pentene (trans)
	TRANS-3,4-DIMETHYL-2-PENTENE
Inchi:	InChI=1S/C7H14/c1-5-7(4)6(2)3/h5-6H,1-4H3/b7-5+
InchiKey:	PPBWEVVDSRKEIK-FNORWQNLSA-N
Formula:	C7H14
SMILES:	CC=C(C)C(C)C
Mol. weight [g/mol]:	98.19
CAS:	4914-92-5

Physical Properties

Property code	Value	Unit	Source
gf	77.29	kJ/mol	Joback Method
hf	-85.66	kJ/mol	Joback Method
hfus	9.25	kJ/mol	Joback Method
hvap	35.10	kJ/mol	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.609		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	677.40		NIST Webbook
rinpol	685.10		NIST Webbook
rinpol	685.80		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	678.70		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	679.40		NIST Webbook
rinpol	679.90		NIST Webbook
rinpol	679.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	680.70		NIST Webbook
rinpol	678.10		NIST Webbook
rinpol	683.00		NIST Webbook

rinpol	683.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	679.00		NIST Webbook
rinpol	681.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	679.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	677.00		NIST Webbook
rinpol	677.50		NIST Webbook
rinpol	688.60		NIST Webbook
rinpol	677.60		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	679.00		NIST Webbook
rinpol	688.60		NIST Webbook
rinpol	687.60		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	680.00		NIST Webbook
tb	364.65 ± 0.60	K	NIST Webbook
tb	364.15 ± 1.50	K	NIST Webbook
tb	364.75 ± 0.30	K	NIST Webbook
tb	364.70	K	NIST Webbook
tb	364.73 ± 0.30	K	NIST Webbook
tb	364.55 ± 0.50	K	NIST Webbook
tc	543.24	K	Joback Method
tf	159.72 ± 0.06	K	NIST Webbook
tf	159.73 ± 0.04	K	NIST Webbook
tf	159.75 ± 0.02	K	NIST Webbook
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.18	J/mol×K	363.16	Joback Method
cpg	192.45	J/mol×K	393.17	Joback Method
cpg	204.18	J/mol×K	423.19	Joback Method

cpg	215.38	J/mol×K	453.20	Joback Method
cpg	226.07	J/mol×K	483.22	Joback Method
cpg	236.27	J/mol×K	513.23	Joback Method
cpg	246.01	J/mol×K	543.24	Joback Method
hvapt	33.90	kJ/mol	353.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38726e+01
Coeff. B	-2.89366e+03
Coeff. C	-5.19180e+01
Temperature range (K), min.	264.92
Temperature range (K), max.	389.92

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=244

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4914925&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity

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

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