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

Other names:	(E)-(CH3)2CHCH=CHCH3
	(E)-4-METHYL-2-PENTENE
	(E)-4-methylpent-2-ene
	4-METHYL-TRANS-2-PENTENE
	4-Methyl-2-pentene, (E)-
	4-Methyl-2-pentene, trans-
	4-Methylpentene-2, trans-
	TRANS-4-METHYL-2-PENTENE
Inchi:	InChI=1S/C6H12/c1-4-5-6(2)3/h4-6H,1-3H3/b5-4+
InchiKey:	LGAQJENWWYGFSN-SNAWJCMRSA-N
Formula:	C6H12
SMILES:	CC=CC(C)C
Mol. weight [g/mol]:	84.16
CAS:	674-76-0

Physical Properties

Property code	Value	Unit	Source
af	0.2900		KDB
gf	79.67	kJ/mol	KDB
hcg	3984.59	kJ/mol	KDB
hcn	3720.496	kJ/mol	KDB
hf	-61.50	kJ/mol	KDB
hfus	7.98	kJ/mol	Joback Method
hvap	30.00	kJ/mol	NIST Webbook
hvap	30.00	kJ/mol	NIST Webbook
hvap	30.00	kJ/mol	NIST Webbook
ie	8.97 ± 0.01	eV	NIST Webbook
ie	8.91	eV	NIST Webbook
ie	8.97 ± 0.01	eV	NIST Webbook
log10ws	-1.95		Crippen Method
logp	2.219		Crippen Method
mcvol	91.100	ml/mol	McGowan Method
pc	3040.00	kPa	KDB
rinpol	562.00		NIST Webbook
rinpol	562.00		NIST Webbook
rinpol	575.50		NIST Webbook
rinpol	574.00		NIST Webbook

rinpol	570.40	NIST Webbook
rinpol	561.70	NIST Webbook
rinpol	570.00	NIST Webbook
rinpol	573.00	NIST Webbook
rinpol	570.40	NIST Webbook
rinpol	561.90	NIST Webbook
rinpol	569.00	NIST Webbook
rinpol	569.00	NIST Webbook
rinpol	569.00	NIST Webbook
rinpol	561.70	NIST Webbook
rinpol	569.10	NIST Webbook
rinpol	568.80	NIST Webbook
rinpol	562.10	NIST Webbook
rinpol	561.90	NIST Webbook
rinpol	570.00	NIST Webbook
rinpol	570.00	NIST Webbook
rinpol	563.00	NIST Webbook
rinpol	563.00	NIST Webbook
rinpol	561.90	NIST Webbook
rinpol	562.00	NIST Webbook
rinpol	561.80	NIST Webbook
rinpol	565.80	NIST Webbook
rinpol	562.00	NIST Webbook
rinpol	562.00	NIST Webbook
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rinpol	575.00		NIST Webbook
rinpol	568.00		NIST Webbook
rinpol	559.00		NIST Webbook
ripol	592.00		NIST Webbook
ripol	590.00		NIST Webbook
ripol	592.00		NIST Webbook
tb	331.70	K	KDB
tc	493.00	K	KDB
tf	132.00	K	KDB
vc	0.360	m3/kmol	KDB
zc	0.2669880		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.87	J/mol×K	458.14	Joback Method
cpg	202.31	J/mol×K	517.01	Joback Method
cpg	193.79	J/mol×K	487.57	Joback Method
cpg	144.81	J/mol×K	340.40	Joback Method
cpg	155.51	J/mol×K	369.83	Joback Method
cpg	165.74	J/mol×K	399.27	Joback Method
cpg	175.52	J/mol×K	428.70	Joback Method
dvisc	0.0003486	Pa×s	272.70	Joback Method
dvisc	0.0001822	Pa×s	340.40	Joback Method
dvisc	0.0002432	Pa×s	306.55	Joback Method
dvisc	0.0086948	Pa×s	137.30	Joback Method
dvisc	0.0024144	Pa×s	171.15	Joback Method
dvisc	0.0010236	Pa×s	205.00	Joback Method
dvisc	0.0005535	Pa×s	238.85	Joback Method
hvapt	31.20	kJ/mol	303.00	NIST Webbook
hvapt	27.95	kJ/mol	331.70	KDB
rfi	1.38583		298.15	KDB
rhol	669.00	kg/m3	293.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41425e+01
Coeff. B	-2.82675e+03
Coeff. C	-3.49530e+01
Temperature range (K), min.	238.98
Temperature range (K), max.	355.05

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.48595e+01
Coeff. B	-5.97972e+03
Coeff. C	-9.14972e+00
Coeff. D	8.09678e-06
Temperature range (K), min.	132.35
Temperature range (K), max.	501.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=208
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=208
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C674760&Units=SI
Measurements of activity coefficients at infinite dilution for organic solutes in two quaternary ammonium-based ionic liquids [DDA][ClO4] and [DDA][BF4]:	https://www.doi.org/10.1016/j.fluid.2018.11.011
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
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
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
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility