1-Pentene, 2-methyl-

Other names:	2-Methyl-1-pentene
	2-Methyl-pentene-1
	2-Methylpentene
	2-methylpent-1-ene
	4-METHYL-4-PENTENE
	C2H5CH2C(CH3)=CH2
Inchi:	InChI=1S/C6H12/c1-4-5-6(2)3/h2,4-5H2,1,3H3
InchiKey:	WWUVJRULCWHUSA-UHFFFAOYSA-N
Formula:	C6H12
SMILES:	C=C(C)CCC
Mol. weight [g/mol]:	84.16
CAS:	763-29-1

Physical Properties

Property code	Value	Unit	Source
af	0.2670		KDB
gf	78.93	kJ/mol	Joback Method
hcg	3986.18	kJ/mol	KDB
hcn	3722.086	kJ/mol	KDB
hf	-51.53	kJ/mol	Joback Method
hfus	8.71	kJ/mol	Joback Method
hvap	30.50	kJ/mol	NIST Webbook
hvap	30.50	kJ/mol	NIST Webbook
hvap	30.50	kJ/mol	NIST Webbook
ie	9.08 ± 0.01	eV	NIST Webbook
ie	9.04	eV	NIST Webbook
ie	9.08 ± 0.01	eV	NIST Webbook
log10ws	-3.03		Estimated Solubility Method
log10ws	-3.03		Aqueous Solubility Prediction Method
logp	2.363		Crippen Method
mcvol	91.100	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=1)		KDB
pc	3280.00	kPa	KDB
rinpol	588.60		NIST Webbook

rinpol	580.90	NIST Webbook
rinpol	588.00	NIST Webbook
rinpol	588.00	NIST Webbook
rinpol	592.40	NIST Webbook
rinpol	592.40	NIST Webbook
rinpol	592.40	NIST Webbook
rinpol	592.40	NIST Webbook
rinpol	592.50	NIST Webbook
rinpol	592.60	NIST Webbook
rinpol	588.00	NIST Webbook
rinpol	585.00	NIST Webbook
rinpol	589.00	NIST Webbook
rinpol	587.70	NIST Webbook
rinpol	588.10	NIST Webbook
rinpol	580.30	NIST Webbook
rinpol	589.00	NIST Webbook
rinpol	589.50	NIST Webbook
rinpol	590.00	NIST Webbook
rinpol	588.80	NIST Webbook
rinpol	588.80	NIST Webbook
rinpol	588.30	NIST Webbook
rinpol	588.00	NIST Webbook
rinpol	587.70	NIST Webbook
rinpol	587.60	NIST Webbook
rinpol	582.00	NIST Webbook
rinpol	580.10	NIST Webbook
rinpol	579.80	NIST Webbook
rinpol	580.30	NIST Webbook
rinpol	581.00	NIST Webbook
rinpol	580.00	NIST Webbook
rinpol	580.20	NIST Webbook
rinpol	580.00	NIST Webbook
rinpol	581.00	NIST Webbook
rinpol	579.25	NIST Webbook
rinpol	588.00	NIST Webbook
rinpol	579.00	NIST Webbook
rinpol	579.00	NIST Webbook
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rinpol	589.00	NIST Webbook
rinpol	575.00	NIST Webbook
rinpol	590.20	NIST Webbook

rinpol	590.00	NIST Webbook
rinpol	584.20	NIST Webbook
rinpol	587.40	NIST Webbook
rinpol	588.00	NIST Webbook
rinpol	583.35	NIST Webbook
rinpol	583.43	NIST Webbook
rinpol	583.00	NIST Webbook
rinpol	588.10	NIST Webbook
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rinpol	579.40		NIST Webbook
rinpol	588.00		NIST Webbook
rinpol	579.60		NIST Webbook
rinpol	587.50		NIST Webbook
ripol	623.00		NIST Webbook
ripol	634.00		NIST Webbook
ripol	634.00		NIST Webbook
tb	335.30	K	KDB
tc	521.00	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tc	506.50	K	KDB
tf	137.00	K	KDB
tf	137.25	K	Aqueous Solubility Prediction Method
tf	137.43 ± 0.40	K	NIST Webbook
vc	0.353	m3/kmol	KDB
zc	0.2753260		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	174.84	J/mol×K	418.33	Joback Method
cpg	183.77	J/mol×K	446.69	Joback Method
cpg	192.34	J/mol×K	475.05	Joback Method
cpg	145.82	J/mol×K	333.24	Joback Method
cpg	155.88	J/mol×K	361.60	Joback Method
cpg	165.55	J/mol×K	389.96	Joback Method
cpg	200.57	J/mol×K	503.41	Joback Method
hvapt	28.07	kJ/mol	335.30	KDB
hvapt	31.60	kJ/mol	306.50	NIST Webbook
rfi	1.38912		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40283e+01
Coeff. B	-2.80476e+03
Coeff. C	-3.71870e+01
Temperature range (K), min.	241.31
Temperature range (K), max.	358.95

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.36898e+01
Coeff. B	-6.02144e+03
Coeff. C	-8.92966e+00
Coeff. D	7.24925e-06
Temperature range (K), min.	137.42
Temperature range (K), max.	507.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=201
Vapor-liquid equilibria of binary mixtures of propylene oxide witheither ethyl benzene, 2-methylpentane, or 2-methyl-1-pentene:	https://www.doi.org/10.1016/j.fluid.2013.04.008
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C763291&Units=SI
KDB:	https://www.cheric.org/files/research/kdb/mol/mol201.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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