1-Pentene, 2,4,4-trimethyl-

Other names:	(tert-C4H9)CH2C(CH3)=CH2
	.alpha.-diisobutylene
	1-Pentene, 2,2,4-trimethyl-
	2,2,4-TRIMETHYL-4-PENETEN
	2,2,4-Trimethyl-4-pentene
	2,4,4-Trimethyl-1-pentene
	2,4,4-Trimethylpent-1-ene
	2,4,4-Trimethylpentene-1
	DIISOBUTENE
	DIISOBUTYLENE
Inchi:	InChI=1S/C8H16/c1-7(2)6-8(3,4)5/h1,6H2,2-5H3
InchiKey:	FXNDIJDIPNCZQJ-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	C=C(C)CC(C)(C)C
Mol. weight [g/mol]:	112.21
CAS:	107-39-1

Physical Properties

Property code	Value	Unit	Source
chl	-5289.08 ± 0.67	kJ/mol	NIST Webbook
chl	-5292.72	kJ/mol	NIST Webbook
gf	98.61	kJ/mol	Joback Method
hf	-101.56	kJ/mol	Joback Method
hfus	6.47	kJ/mol	Joback Method
hvap	35.70	kJ/mol	NIST Webbook
hvap	35.70	kJ/mol	NIST Webbook
hvap	35.70	kJ/mol	NIST Webbook
ie	8.91 ± 0.01	eV	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
rinpol	708.00		NIST Webbook
rinpol	716.80		NIST Webbook
rinpol	710.20		NIST Webbook
rinpol	711.50		NIST Webbook
rinpol	711.90		NIST Webbook

rinpol	712.60		NIST Webbook
rinpol	717.10		NIST Webbook
rinpol	714.30		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	715.30		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	703.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	709.00		NIST Webbook
rinpol	709.00		NIST Webbook
rinpol	713.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	716.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	703.00		NIST Webbook
rinpol	709.00		NIST Webbook
rinpol	713.80		NIST Webbook
rinpol	711.20		NIST Webbook
rinpol	709.90		NIST Webbook
rinpol	717.60		NIST Webbook
rinpol	715.20		NIST Webbook
rinpol	714.00		NIST Webbook
rinpol	713.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	701.50		NIST Webbook
rinpol	708.60		NIST Webbook
rinpol	716.40		NIST Webbook
rinpol	712.50		NIST Webbook
ripol	750.00		NIST Webbook
ripol	750.00		NIST Webbook
sl	311.70	J/mol×K	NIST Webbook

sl	306.30	J/mol×K	NIST Webbook
tb	375.00 ± 3.00	K	NIST Webbook
tb	375.80 ± 0.50	K	NIST Webbook
tb	378.10 ± 0.50	K	NIST Webbook
tb	374.60	K	NIST Webbook
tb	373.25 ± 0.30	K	NIST Webbook
tb	374.40 ± 0.50	K	NIST Webbook
tb	375.95 ± 0.30	K	NIST Webbook
tb	374.40 ± 0.60	K	NIST Webbook
tb	374.40 ± 1.00	K	NIST Webbook
tb	374.59 ± 0.20	K	NIST Webbook
tb	374.59 ± 0.20	K	NIST Webbook
tb	374.59 ± 0.20	K	NIST Webbook
tb	374.59 ± 0.30	K	NIST Webbook
tb	374.70 ± 0.15	K	NIST Webbook
tb	374.80 ± 0.15	K	NIST Webbook
tb	374.70 ± 0.60	K	NIST Webbook
tb	374.45 ± 0.30	K	NIST Webbook
tb	374.60 ± 0.50	K	NIST Webbook
tb	377.61 ± 2.00	K	NIST Webbook
tb	374.58 ± 0.05	K	NIST Webbook
tb	375.00 ± 3.00	K	NIST Webbook
tc	557.27	K	Joback Method
tf	166.62	K	Joback Method
tt	178.90 ± 0.20	K	NIST Webbook
tt	172.00 ± 1.00	K	NIST Webbook
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.42	J/mol×K	557.27	Joback Method
cpg	218.61	J/mol×K	375.77	Joback Method
cpg	283.40	J/mol×K	527.02	Joback Method
cpg	271.77	J/mol×K	496.77	Joback Method
cpg	259.50	J/mol×K	466.52	Joback Method
cpg	246.58	J/mol×K	436.27	Joback Method
cpg	232.95	J/mol×K	406.02	Joback Method
cpl	240.20	J/mol×K	298.60	NIST Webbook
cpl	235.35	J/mol×K	296.00	NIST Webbook
hfust	8.77	kJ/mol	178.90	NIST Webbook

hfust	8.79	kJ/mol	178.90	NIST Webbook
hfust	6.79	kJ/mol	166.00	NIST Webbook
hfust	8.77	kJ/mol	178.90	NIST Webbook
hvapt	33.50	kJ/mol	362.00	NIST Webbook
hvapt	35.10	kJ/mol	338.00	NIST Webbook
pvap	47.01	kPa	349.50	Vapor-Liquid Equilibrium for Benzaldehyde with 1-Methylethylbenzene and for 2-Methyl-propan-2-ol with 2,4,4-Trimethyl-1-pentene
pvap	53.00	kPa	353.14	Vapor-Liquid Equilibrium for Benzaldehyde with 1-Methylethylbenzene and for 2-Methyl-propan-2-ol with 2,4,4-Trimethyl-1-pentene
pvap	58.57	kPa	356.24	Vapor-Liquid Equilibrium for Benzaldehyde with 1-Methylethylbenzene and for 2-Methyl-propan-2-ol with 2,4,4-Trimethyl-1-pentene
pvap	20.63	kPa	326.72	Vapor-Liquid Equilibrium for Benzaldehyde with 1-Methylethylbenzene and for 2-Methyl-propan-2-ol with 2,4,4-Trimethyl-1-pentene
pvap	42.90	kPa	346.79	Vapor-Liquid Equilibrium for Benzaldehyde with 1-Methylethylbenzene and for 2-Methyl-propan-2-ol with 2,4,4-Trimethyl-1-pentene
pvap	37.81	kPa	343.12	Vapor-Liquid Equilibrium for Benzaldehyde with 1-Methylethylbenzene and for 2-Methyl-propan-2-ol with 2,4,4-Trimethyl-1-pentene

pvap	33.57	kPa	339.75	Vapor-Liquid Equilibrium for Benzaldehyde with 1-Methylethylbenzene and for 2-Methyl-propan-2-ol with 2,4,4-Trimethyl-1-pentene
pvap	29.75	kPa	336.41	Vapor-Liquid Equilibrium for Benzaldehyde with 1-Methylethylbenzene and for 2-Methyl-propan-2-ol with 2,4,4-Trimethyl-1-pentene
pvap	8.66	kPa	306.23	Vapor-Liquid Equilibrium for Benzaldehyde with 1-Methylethylbenzene and for 2-Methyl-propan-2-ol with 2,4,4-Trimethyl-1-pentene
pvap	10.15	kPa	309.74	Vapor-Liquid Equilibrium for Benzaldehyde with 1-Methylethylbenzene and for 2-Methyl-propan-2-ol with 2,4,4-Trimethyl-1-pentene
pvap	11.78	kPa	313.14	Vapor-Liquid Equilibrium for Benzaldehyde with 1-Methylethylbenzene and for 2-Methyl-propan-2-ol with 2,4,4-Trimethyl-1-pentene
pvap	13.56	kPa	316.42	Vapor-Liquid Equilibrium for Benzaldehyde with 1-Methylethylbenzene and for 2-Methyl-propan-2-ol with 2,4,4-Trimethyl-1-pentene
pvap	26.37	kPa	333.14	Vapor-Liquid Equilibrium for Benzaldehyde with 1-Methylethylbenzene and for 2-Methyl-propan-2-ol with 2,4,4-Trimethyl-1-pentene

pvap	17.94	kPa	323.20	Vapor-Liquid Equilibrium for Benzaldehyde with 1-Methylethylbenzene and for 2-Methyl-propan-2-ol with 2,4,4-Trimethyl-1-pentene
pvap	23.47	kPa	330.07	Vapor-Liquid Equilibrium for Benzaldehyde with 1-Methylethylbenzene and for 2-Methyl-propan-2-ol with 2,4,4-Trimethyl-1-pentene
pvap	15.49	kPa	319.61	Vapor-Liquid Equilibrium for Benzaldehyde with 1-Methylethylbenzene and for 2-Methyl-propan-2-ol with 2,4,4-Trimethyl-1-pentene
rfi	1.40620		298.15	Phase equilibria on four binary systems containing 3-methylthiophene
rhol	710.73	kg/m3	298.15	Binary Liquid Liquid Equilibria of ?-Valerolactone with Some Hydrocarbons
rhol	710.70	kg/m3	298.15	Measurements and modeling of LLE and HE for (methanol + 2,4,4-trimethyl-1-pentene), and LLE for (water + methanol + 2,4,4-trimethyl-1-pentene)
sfust	40.90	J/mol×K	166.00	NIST Webbook
sfust	48.99	J/mol×K	178.90	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbp	374.50	K	101.20	Vapor Liquid Equilibria for Ethanol + 2,4,4-Trimethyl-1-pentene and 2-Propanol + 2,4,4-Trimethyl-1-pentene at 101 kPa

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38710e+01
Coeff. B	-3.06177e+03
Coeff. C	-4.40930e+01
Temperature range (K), min.	269.50
Temperature range (K), max.	401.80

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.30325e+01
Coeff. B	-6.61504e+03
Coeff. C	-8.69861e+00
Coeff. D	5.59308e-06
Temperature range (K), min.	179.70
Temperature range (K), max.	553.00

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Vapor-Liquid Equilibrium for Benzaldehyde with 1-Methylethylbenzene and for 2-Methyl-propan-2-ol with 2,4,4-Trimethyl-1-pentene:	https://www.doi.org/10.1021/je060359o
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107391&Units=SI
Vapor-Liquid Equilibrium Data at 343 K and Excess Molar Enthalpy Data at 298 K for the Binary Systems of Ethanol + 2,4,4-Trimethyl-1-pentene and 2-Propanol + 2,4,4-Trimethyl-1-pentene:	https://www.doi.org/10.1021/je025556b
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Vapor-liquid equilibrium for binary system of tetrahydrothiophene + 2,2,4-trimethylpentane and tetrahydrothiophene + 2,4,4-trimethyl-1-pentene at 358.15 K and 368.15 K:	https://www.doi.org/10.1016/j.fluid.2010.03.022
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=329
Vapor-Liquid Equilibria for Ethanol + 2,4,4-Trimethyl-1-pentene and 2-Propanol + 2,4,4-Trimethyl-1-pentene at 101 kPa:	https://www.doi.org/10.1021/je020105c

Phase equilibria for systems containing dimethyl disulfide and diethyl disulfide with hydrocarbons at 303.15 K:	https://www.doi.org/10.1016/j.fluid.2010.02.043
Infinite dilution activity coefficient and vapour liquid equilibrium measurements for dimethylsulphide and tetrahydrothiophene with hydrocarbons:	https://www.doi.org/10.1016/j.fluid.2010.03.027
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol329.mol
Phase equilibria on four binary systems containing 3-methylthiophene:	https://www.doi.org/10.1016/j.fluid.2009.02.010
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Measurements and modeling of LLE and HE for (methanol + 2,4,4-trimethyl-1-pentene), and LLE for (water + methanol + 2,4,4-trimethyl-1-pentene):	https://www.doi.org/10.1016/j.jct.2015.01.013
Binary Liquid-Liquid Equilibria of γ-Valerolactone with Some Hydrocarbons:	https://www.doi.org/10.1021/je501074b
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume