Pentane, 2,2,4,4-tetramethyl-

Other names: 2,2,4,4-Tetramethylpentane
DI-TERT-BUTYLMETHANE
Inchi: InChI=1S/C9H20/c1-8(2,3)7-9(4,5)6/h7H2,1-6H3
InchiKey: GUMULFRCHLJNDY-UHFFFAOYSA-N
Formula: C9H20
SMILES: CC(C)(C)CC(C)(C)C
Mol. weight [g/mol]: 128.26
CAS: 1070-87-7

Physical Properties

Property code	Value	Unit	Source
af	0.3120		KDB
ap	348.150	K	KDB
chl	-6117.80	kJ/mol	NIST Webbook
chl	-6118.70	kJ/mol	NIST Webbook
chl	-6119.90 ± 1.30	kJ/mol	NIST Webbook
gf	34.04	kJ/mol	KDB
hcg	6119.90	kJ/mol	KDB
hcn	5679.780	kJ/mol	KDB
hf	-242.10	kJ/mol	KDB
hf	-241.50 ± 1.50	kJ/mol	NIST Webbook
hfus	4.24	kJ/mol	Joback Method
hvap	38.55	kJ/mol	NIST Webbook
hvap	38.20	kJ/mol	NIST Webbook
hvap	38.50 ± 0.30	kJ/mol	NIST Webbook
hvap	38.50 ± 0.10	kJ/mol	NIST Webbook
hvap	38.50 ± 0.30	kJ/mol	NIST Webbook
log10ws	-3.11		Crippen Method
logp	3.469		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
pc	2490.00 ± 40.00	kPa	NIST Webbook
pc	2485.00 ± 10.00	kPa	NIST Webbook
pc	2490.00	kPa	KDB
rinpol	771.00		NIST Webbook
rinpol	776.90		NIST Webbook
rinpol	820.80		NIST Webbook
rinpol	766.00		NIST Webbook

rinpol	769.00	NIST Webbook
rinpol	819.40	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	774.60	NIST Webbook
rinpol	772.30	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	769.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	769.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	772.30	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	769.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	769.00	NIST Webbook

rinpol	768.00		NIST Webbook
sg	430.16	J/mol×K	NIST Webbook
sl	331.80	J/mol×K	NIST Webbook
tb	395.44	K	KDB
tc	574.60	K	KDB
tc	574.60 ± 0.50	K	NIST Webbook
tc	574.65 ± 0.10	K	NIST Webbook
tf	206.61 ± 0.06	K	NIST Webbook
tf	206.61	K	KDB
tf	208.15 ± 2.00	K	NIST Webbook
tf	207.95 ± 0.60	K	NIST Webbook
tf	206.61 ± 0.06	K	NIST Webbook
tf	206.15 ± 0.30	K	NIST Webbook
tf	206.55 ± 0.15	K	NIST Webbook
tt	206.61 ± 0.02	K	NIST Webbook
vc	0.504	m3/kmol	KDB
zc	0.2626800		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.44	J/mol×K	491.36	Joback Method
cpg	308.94	J/mol×K	460.53	Joback Method
cpg	365.94	J/mol×K	583.86	Joback Method
cpg	352.90	J/mol×K	553.03	Joback Method
cpg	339.09	J/mol×K	522.19	Joback Method
cpg	275.15	J/mol×K	398.86	Joback Method
cpg	292.52	J/mol×K	429.69	Joback Method
cpl	266.30	J/mol×K	298.15	NIST Webbook
dvisc	0.0006761	Pa×s	331.25	Joback Method
dvisc	0.0011864	Pa×s	297.44	Joback Method
dvisc	0.0205234	Pa×s	196.03	Joback Method
dvisc	0.0060005	Pa×s	229.84	Joback Method
dvisc	0.0024048	Pa×s	263.64	Joback Method
dvisc	0.0002923	Pa×s	398.86	Joback Method
dvisc	0.0004276	Pa×s	365.06	Joback Method
hfust	9.75	kJ/mol	206.70	NIST Webbook
hfust	9.74	kJ/mol	206.61	NIST Webbook
hfust	9.75	kJ/mol	206.70	NIST Webbook
hvapt	32.84	kJ/mol	395.40	KDB
hvapt	34.80	kJ/mol	398.50	NIST Webbook

hvapt	36.50	kJ/mol	353.00	NIST Webbook
hvapt	37.20	kJ/mol	355.00	NIST Webbook
hvapt	32.51	kJ/mol	395.50	NIST Webbook
rfi	1.40459		298.15	KDB
rhol	719.00	kg/m3	293.00	KDB
sfust	47.16	J/mol×K	206.61	NIST Webbook
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40474e+01
Coeff. B	-3.30866e+03
Coeff. C	-4.45400e+01
Temperature range (K), min.	285.00
Temperature range (K), max.	423.28

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.55763e+01
Coeff. B	-7.01322e+03
Coeff. C	-9.05593e+00
Coeff. D	5.95333e-06
Temperature range (K), min.	206.95
Temperature range (K), max.	571.35

Sources

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=96
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/files/research/kdb/mol/mol96.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1070877&Units=SI

Legend

af:	Acentric Factor
ap:	Aniline Point
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hfust:	Enthalpy of fusion at a given temperature
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
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility