Pentane, 3,3-dimethyl-

Other names: (C2H5)2C(CH3)2
3,3-Dimethylpentane
Inchi: InChI=1S/C7H16/c1-5-7(3,4)6-2/h5-6H2,1-4H3
InchiKey: AEXMKKGTQYQZCS-UHFFFAOYSA-N
Formula: C7H16
SMILES: CCC(C)(C)CC
Mol. weight [g/mol]: 100.20
CAS: 562-49-2

Physical Properties

Property code	Value	Unit	Source
af	0.2670		KDB
ap	343.650	K	KDB
chl	-4806.70 ± 0.79	kJ/mol	NIST Webbook
chl	-4802.00 ± 1.00	kJ/mol	NIST Webbook
dm	0.00	debye	KDB
gf	2.64	kJ/mol	KDB
hcg	4806.70	kJ/mol	KDB
hcn	4454.580	kJ/mol	KDB
hf	-201.70	kJ/mol	KDB
hf	-205.90	kJ/mol	NIST Webbook
hf	-201.50 ± 0.92	kJ/mol	NIST Webbook
hfl	-239.00 ± 1.00	kJ/mol	NIST Webbook
hfl	-234.60 ± 0.92	kJ/mol	NIST Webbook
hfus	6.47	kJ/mol	Joback Method
hvap	33.00	kJ/mol	NIST Webbook
hvap	33.15	kJ/mol	NIST Webbook
hvap	33.00 ± 0.10	kJ/mol	NIST Webbook
hvap	33.00 ± 0.10	kJ/mol	NIST Webbook
hvap	33.02	kJ/mol	NIST Webbook
log10ws	-4.23		Aqueous Solubility Prediction Method
log10ws	-4.23		Estimated Solubility Method
logp	2.833		Crippen Method
mcvol	109.490	ml/mol	McGowan Method
pc	2945.80 ± 40.53	kPa	NIST Webbook
pc	2950.00	kPa	KDB

pc	2950.00 ± 50.00	kPa	NIST Webbook
rhoc	242.49 ± 5.01	kg/m3	NIST Webbook
rhoc	242.49 ± 5.01	kg/m3	NIST Webbook
rinpol	646.00		NIST Webbook
rinpol	649.00		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	653.00		NIST Webbook
rinpol	659.00		NIST Webbook
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rinpol	660.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	647.00		NIST Webbook
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rinpol	648.00		NIST Webbook
rinpol	647.32		NIST Webbook
rinpol	647.31		NIST Webbook
rinpol	650.50		NIST Webbook
rinpol	651.50		NIST Webbook
rinpol	644.47		NIST Webbook
rinpol	643.69		NIST Webbook
rinpol	651.90		NIST Webbook
rinpol	654.25		NIST Webbook
rinpol	657.00		NIST Webbook
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rinpol	661.00		NIST Webbook
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rinpol	662.00		NIST Webbook
rinpol	659.00		NIST Webbook

rinpol	656.00	NIST Webbook
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rinpol	662.00	NIST Webbook
rinpol	656.00	NIST Webbook
rinpol	660.00	NIST Webbook
rinpol	659.10	NIST Webbook
rinpol	660.00	NIST Webbook
rinpol	658.00	NIST Webbook
rinpol	657.00	NIST Webbook
rinpol	656.00	NIST Webbook
rinpol	654.00	NIST Webbook
rinpol	662.46	NIST Webbook
rinpol	660.59	NIST Webbook
rinpol	667.80	NIST Webbook
rinpol	665.95	NIST Webbook
rinpol	664.21	NIST Webbook
rinpol	662.00	NIST Webbook
rinpol	646.00	NIST Webbook
rinpol	657.00	NIST Webbook
rinpol	658.00	NIST Webbook
rinpol	653.00	NIST Webbook
rinpol	669.00	NIST Webbook
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rinpol	654.25	NIST Webbook
rinpol	651.00	NIST Webbook
rinpol	662.00	NIST Webbook
rinpol	650.00	NIST Webbook
rinpol	664.00	NIST Webbook
rinpol	653.00	NIST Webbook
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rinpol	669.00	NIST Webbook
rinpol	653.10	NIST Webbook
rinpol	656.30	NIST Webbook
rinpol	660.00	NIST Webbook
rinpol	649.00	NIST Webbook
rinpol	662.80	NIST Webbook
rinpol	658.00	NIST Webbook
rinpol	656.00	NIST Webbook
rinpol	658.10	NIST Webbook
rinpol	658.00	NIST Webbook

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rinpol	661.50	NIST Webbook
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rinpol	661.20	NIST Webbook
rinpol	654.70	NIST Webbook
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rinpol	658.00	NIST Webbook
rinpol	659.70	NIST Webbook
rinpol	661.40	NIST Webbook
rinpol	663.40	NIST Webbook
rinpol	657.00	NIST Webbook
rinpol	657.60	NIST Webbook
rinpol	657.90	NIST Webbook
rinpol	658.30	NIST Webbook
rinpol	658.80	NIST Webbook
rinpol	659.30	NIST Webbook

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rinpol	662.00		NIST Webbook
rinpol	663.00		NIST Webbook
rinpol	657.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	652.00		NIST Webbook
sg	398.02	J/mol×K	NIST Webbook
sl	293.30	J/mol×K	NIST Webbook
sl	305.60	J/mol×K	NIST Webbook
tb	359.25 ± 0.20	K	NIST Webbook
tb	359.21	K	KDB
tb	359.30	K	NIST Webbook
tb	359.20	K	NIST Webbook
tb	359.15 ± 0.40	K	NIST Webbook
tb	359.21 ± 0.20	K	NIST Webbook
tb	359.22 ± 0.20	K	NIST Webbook
tb	359.20 ± 0.20	K	NIST Webbook
tb	359.20 ± 0.20	K	NIST Webbook
tb	359.20 ± 0.30	K	NIST Webbook
tb	359.20 ± 0.20	K	NIST Webbook
tb	359.25 ± 0.50	K	NIST Webbook
tb	358.95 ± 0.40	K	NIST Webbook
tb	359.25 ± 0.30	K	NIST Webbook
tb	359.20 ± 0.20	K	NIST Webbook
tb	359.25 ± 0.30	K	NIST Webbook
tb	359.21 ± 0.01	K	NIST Webbook
tb	359.24 ± 0.20	K	NIST Webbook
tb	359.25 ± 0.30	K	NIST Webbook
tb	363.05 ± 0.50	K	NIST Webbook
tb	363.15 ± 0.50	K	NIST Webbook
tb	359.23 ± 0.30	K	NIST Webbook
tb	359.21 ± 0.06	K	NIST Webbook
tb	359.00 ± 0.30	K	NIST Webbook
tb	359.12 ± 0.10	K	NIST Webbook
tb	359.00 ± 0.50	K	NIST Webbook
tb	359.25 ± 0.50	K	NIST Webbook
tb	359.25 ± 0.30	K	NIST Webbook
tb	360.00 ± 3.00	K	NIST Webbook
tb	359.70 ± 2.00	K	NIST Webbook
tb	359.40 ± 0.60	K	NIST Webbook
tb	359.15 ± 0.50	K	NIST Webbook
tb	359.15 ± 0.50	K	NIST Webbook

tb	359.10 ± 0.50	K	NIST Webbook
tb	359.25 ± 0.30	K	NIST Webbook
tb	359.25 ± 0.20	K	NIST Webbook
tb	359.15 ± 0.50	K	NIST Webbook
tb	359.25 ± 0.30	K	NIST Webbook
tb	359.21 ± 0.10	K	NIST Webbook
tc	536.40	K	KDB
tc	536.30	K	NIST Webbook
tc	536.34 ± 0.40	K	NIST Webbook
tc	536.40 ± 0.50	K	NIST Webbook
tf	138.15 ± 0.30	K	NIST Webbook
tf	138.34 ± 0.30	K	NIST Webbook
tf	137.54 ± 0.50	K	NIST Webbook
tf	138.70 ± 0.05	K	NIST Webbook
tf	138.52	K	Aqueous Solubility Prediction Method
tf	138.70 ± 0.05	K	NIST Webbook
tf	138.71 ± 0.05	K	NIST Webbook
tf	138.17 ± 0.30	K	NIST Webbook
tf	138.17 ± 0.20	K	NIST Webbook
tf	137.60 ± 0.40	K	NIST Webbook
tf	138.16 ± 0.01	K	NIST Webbook
tf	138.64 ± 0.06	K	NIST Webbook
tf	138.64 ± 0.05	K	NIST Webbook
tf	138.20	K	KDB
tf	138.69 ± 0.04	K	NIST Webbook
tf	138.25 ± 0.50	K	NIST Webbook
tf	137.59 ± 0.05	K	NIST Webbook
tf	138.12 ± 0.50	K	NIST Webbook
tf	137.50 ± 0.30	K	NIST Webbook
tf	137.55 ± 0.70	K	NIST Webbook
tf	137.24 ± 0.40	K	NIST Webbook
tf	137.41 ± 0.20	K	NIST Webbook
tf	137.45 ± 0.30	K	NIST Webbook
tf	137.45 ± 0.50	K	NIST Webbook
tf	138.15 ± 0.50	K	NIST Webbook
tf	138.20 ± 0.05	K	NIST Webbook
tf	138.15 ± 0.50	K	NIST Webbook
tt	138.75 ± 0.10	K	NIST Webbook
tt	138.20 ± 0.03	K	NIST Webbook
tt	138.20 ± 0.20	K	NIST Webbook
vc	0.414	m3/kmol	NIST Webbook
vc	0.414	m3/kmol	KDB
zc	0.2738400		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.68 ± 0.40	J/mol×K	366.22	NIST Webbook
cpg	214.51 ± 0.43	J/mol×K	402.31	NIST Webbook
cpg	235.08 ± 0.47	J/mol×K	449.30	NIST Webbook
cpg	250.70 ± 0.50	J/mol×K	487.21	NIST Webbook
cpg	187.44 ± 0.37	J/mol×K	344.13	NIST Webbook
cpl	211.70	J/mol×K	292.90	NIST Webbook
cpl	214.80	J/mol×K	298.15	NIST Webbook
dvisc	0.0017220	Pa×s	232.82	Joback Method
dvisc	0.0005792	Pa×s	294.58	Joback Method
dvisc	0.0112423	Pa×s	171.07	Joback Method
dvisc	0.0002842	Pa×s	356.33	Joback Method
dvisc	0.0038120	Pa×s	201.95	Joback Method
dvisc	0.0009370	Pa×s	263.70	Joback Method
dvisc	0.0003923	Pa×s	325.45	Joback Method
hfust	7.07	kJ/mol	138.20	NIST Webbook
hfust	7.07	kJ/mol	138.20	NIST Webbook
hfust	7.07	kJ/mol	138.20	NIST Webbook
hvapt	33.60	kJ/mol	320.00	NIST Webbook
hvapt	29.65	kJ/mol	359.20	KDB
hvapt	33.30	kJ/mol	322.50	NIST Webbook
hvapt	33.20	kJ/mol	323.50	NIST Webbook
hvapt	34.80	kJ/mol	247.00	NIST Webbook
hvapt	29.62	kJ/mol	359.20	NIST Webbook
rfi	1.38842		298.15	KDB
rhol	693.00	kg/m3	293.00	KDB
sfust	51.14	J/mol×K	138.20	NIST Webbook
srf	0.02	N/m	298.20	KDB
tcondl	0.09	W/m×K	334.37	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)

tcondl	0.10	W/m×K	316.38	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.10	W/m×K	296.63	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.10	W/m×K	296.39	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.10	W/m×K	296.03	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.09	W/m×K	316.93	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.10	W/m×K	296.01	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.11	W/m×K	276.78	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	

tcondl	0.09	W/m×K	316.67	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.11	W/m×K	276.50	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.11	W/m×K	276.17	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.11	W/m×K	257.04	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.11	W/m×K	256.71	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.09	W/m×K	333.75	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	
tcondl	0.09	W/m×K	334.10	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)	

tcondl	0.11	W/m×K	256.11	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42009e+01
Coeff. B	-3.13031e+03
Coeff. C	-3.25430e+01
Temperature range (K), min.	257.53
Temperature range (K), max.	384.68

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.78524e+01
Coeff. B	-6.06498e+03
Coeff. C	-8.01550e+00
Coeff. D	6.29022e-06
Temperature range (K), min.	138.70
Temperature range (K), max.	536.40

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C562492&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=45
Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8):	https://www.doi.org/10.1021/je020125e
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol45.mol

Legend

af:	Acentric Factor
ap:	Aniline Point
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
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
hfl:	Liquid phase 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
rhoc:	Critical density
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
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

zc:	Critical Compressibility
zra:	Rackett Parameter