

Pentane, 2,2-dimethyl-

Other names:	2,2-Dimethylpentane
Inchi:	InChI=1S/C7H16/c1-5-6-7(2,3)4/h5-6H2,1-4H3
InchiKey:	CXOWYJMDMMMMJO-UHFFFAOYSA-N
Formula:	C7H16
SMILES:	CCCC(C)(C)C
Mol. weight [g/mol]:	100.20
CAS:	590-35-2

Physical Properties

Property code	Value	Unit	Source
af	0.2870		KDB
ap	350.750	K	KDB
chl	-4802.60 ± 1.30	kJ/mol	NIST Webbook
chl	-4798.00 ± 1.00	kJ/mol	NIST Webbook
dm	0.00	debye	KDB
gf	0.84	kJ/mol	KDB
hcg	4802.60	kJ/mol	KDB
hcn	4450.479	kJ/mol	KDB
hf	-206.30	kJ/mol	KDB
hf	-209.50	kJ/mol	NIST Webbook
hf	-206.20 ± 1.30	kJ/mol	NIST Webbook
hfl	-238.70 ± 1.30	kJ/mol	NIST Webbook
hfl	-242.00 ± 1.00	kJ/mol	NIST Webbook
hfus	6.47	kJ/mol	Joback Method
hvap	32.20 ± 0.10	kJ/mol	NIST Webbook
hvap	32.40 ± 0.10	kJ/mol	NIST Webbook
hvap	32.40 ± 0.10	kJ/mol	NIST Webbook
hvap	32.42	kJ/mol	NIST Webbook
hvap	32.56	kJ/mol	NIST Webbook
log10ws	-4.36		Estimated Solubility Method
log10ws	-4.36		Aqueous Solubility Prediction Method
logp	2.833		Crippen Method
mcvol	109.490	ml/mol	McGowan Method
pc	2877.63 ± 50.66	kPa	NIST Webbook
pc	2773.00 ± 40.53	kPa	NIST Webbook
pc	2770.00 ± 50.00	kPa	NIST Webbook

pc	2770.00	kPa	KDB
rhoc	241.49 ± 5.01	kg/m3	NIST Webbook
rhoc	241.49 ± 5.01	kg/m3	NIST Webbook
rinpol	627.90		NIST Webbook
rinpol	626.90		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	625.60		NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	625.60		NIST Webbook
rinpol	626.90		NIST Webbook
rinpol	623.80		NIST Webbook
rinpol	624.80		NIST Webbook
rinpol	625.10		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	622.70		NIST Webbook
rinpol	623.20		NIST Webbook
rinpol	623.80		NIST Webbook
rinpol	624.40		NIST Webbook
rinpol	625.10		NIST Webbook
rinpol	625.80		NIST Webbook
rinpol	625.70		NIST Webbook
rinpol	625.60		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	623.40		NIST Webbook
rinpol	624.60		NIST Webbook
rinpol	625.70		NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	628.30		NIST Webbook
rinpol	629.70		NIST Webbook
rinpol	627.20		NIST Webbook
rinpol	626.50		NIST Webbook
rinpol	625.60		NIST Webbook
rinpol	625.00		NIST Webbook

rinpol	624.10	NIST Webbook
rinpol	623.10	NIST Webbook
rinpol	625.00	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	624.00	NIST Webbook
rinpol	625.00	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	627.00	NIST Webbook
rinpol	628.00	NIST Webbook
rinpol	627.00	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	624.20	NIST Webbook
rinpol	625.00	NIST Webbook
rinpol	625.00	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	627.00	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	627.00	NIST Webbook
rinpol	629.70	NIST Webbook
rinpol	630.40	NIST Webbook
rinpol	631.70	NIST Webbook
rinpol	627.79	NIST Webbook
rinpol	628.51	NIST Webbook
rinpol	621.00	NIST Webbook
rinpol	622.00	NIST Webbook
rinpol	623.00	NIST Webbook
rinpol	623.00	NIST Webbook
rinpol	624.00	NIST Webbook
rinpol	625.80	NIST Webbook
rinpol	622.00	NIST Webbook
rinpol	625.00	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	673.00	NIST Webbook
rinpol	624.00	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	627.00	NIST Webbook
rinpol	628.00	NIST Webbook
rinpol	624.50	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	624.00	NIST Webbook
rinpol	625.00	NIST Webbook

rinpol	627.00	NIST Webbook
rinpol	625.00	NIST Webbook
rinpol	625.00	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	625.00	NIST Webbook
rinpol	618.00	NIST Webbook
rinpol	620.00	NIST Webbook
rinpol	624.25	NIST Webbook
rinpol	628.00	NIST Webbook
rinpol	621.40	NIST Webbook
rinpol	615.96	NIST Webbook
rinpol	616.70	NIST Webbook
rinpol	618.20	NIST Webbook
rinpol	620.50	NIST Webbook
rinpol	618.59	NIST Webbook
rinpol	618.60	NIST Webbook
rinpol	619.00	NIST Webbook
rinpol	618.00	NIST Webbook
rinpol	620.00	NIST Webbook
rinpol	624.00	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	624.00	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	629.00	NIST Webbook
rinpol	627.00	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	619.00	NIST Webbook
rinpol	625.00	NIST Webbook
rinpol	622.00	NIST Webbook
rinpol	623.00	NIST Webbook
rinpol	628.00	NIST Webbook
rinpol	619.00	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	669.00	NIST Webbook
rinpol	628.00	NIST Webbook
rinpol	659.00	NIST Webbook
rinpol	627.00	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	620.00	NIST Webbook
rinpol	627.00	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	623.00	NIST Webbook
rinpol	621.00	NIST Webbook

rinpol	622.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	635.00		NIST Webbook
rinpol	659.00		NIST Webbook
rinpol	628.10		NIST Webbook
rinpol	620.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	623.00		NIST Webbook
rinpol	624.25		NIST Webbook
rinpol	624.80		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	625.70		NIST Webbook
rinpol	625.60		NIST Webbook
rinpol	625.70		NIST Webbook
rinpol	625.60		NIST Webbook
rinpol	625.70		NIST Webbook
rinpol	621.80		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	627.70		NIST Webbook
rinpol	624.10		NIST Webbook
rinpol	622.40		NIST Webbook
rinpol	633.00		NIST Webbook
rinpol	626.00		NIST Webbook
sg	392.88	J/mol×K	NIST Webbook
sl	284.90	J/mol×K	NIST Webbook
sl	300.29	J/mol×K	NIST Webbook
tb	352.15 ± 0.50	K	NIST Webbook
tb	352.15 ± 1.00	K	NIST Webbook
tb	352.33 ± 0.20	K	NIST Webbook
tb	352.35 ± 0.20	K	NIST Webbook
tb	352.35 ± 0.30	K	NIST Webbook
tb	352.35 ± 0.01	K	NIST Webbook
tb	352.35 ± 0.50	K	NIST Webbook
tb	352.35 ± 0.30	K	NIST Webbook
tb	352.35 ± 0.20	K	NIST Webbook
tb	352.35 ± 0.20	K	NIST Webbook
tb	352.25 ± 0.50	K	NIST Webbook
tb	352.35 ± 0.20	K	NIST Webbook

tb	352.35 ± 0.05	K	NIST Webbook
tb	352.25 ± 0.30	K	NIST Webbook
tb	352.40 ± 0.50	K	NIST Webbook
tb	352.30	K	KDB
tb	352.40 ± 0.30	K	NIST Webbook
tb	352.00 ± 0.50	K	NIST Webbook
tb	351.95 ± 0.50	K	NIST Webbook
tb	352.45 ± 0.50	K	NIST Webbook
tb	352.36 ± 0.20	K	NIST Webbook
tb	352.45 ± 0.30	K	NIST Webbook
tb	352.36 ± 0.20	K	NIST Webbook
tb	352.45 ± 0.50	K	NIST Webbook
tb	352.25 ± 0.30	K	NIST Webbook
tb	352.45 ± 0.20	K	NIST Webbook
tb	352.05 ± 0.50	K	NIST Webbook
tb	352.05 ± 0.50	K	NIST Webbook
tb	351.95 ± 0.50	K	NIST Webbook
tb	352.45 ± 0.50	K	NIST Webbook
tb	352.05 ± 0.50	K	NIST Webbook
tb	352.05 ± 0.50	K	NIST Webbook
tb	353.65 ± 1.00	K	NIST Webbook
tb	352.45 ± 0.50	K	NIST Webbook
tb	352.45 ± 0.50	K	NIST Webbook
tb	363.15 ± 0.30	K	NIST Webbook
tb	353.96 ± 1.00	K	NIST Webbook
tb	352.40	K	NIST Webbook
tb	352.25 ± 0.50	K	NIST Webbook
tb	352.40	K	NIST Webbook
tb	352.65 ± 0.30	K	NIST Webbook
tb	352.15 ± 0.50	K	NIST Webbook
tb	352.34 ± 0.02	K	NIST Webbook
tb	352.30 ± 0.30	K	NIST Webbook
tb	352.35 ± 0.30	K	NIST Webbook
tb	352.40 ± 0.50	K	NIST Webbook
tb	353.00 ± 2.00	K	NIST Webbook
tb	352.35 ± 0.30	K	NIST Webbook
tb	351.65 ± 1.50	K	NIST Webbook
tb	352.33 ± 0.30	K	NIST Webbook
tb	352.15 ± 0.40	K	NIST Webbook
tb	352.45 ± 0.30	K	NIST Webbook
tb	352.35 ± 0.10	K	NIST Webbook
tb	352.35 ± 0.20	K	NIST Webbook
tc	520.85 ± 0.50	K	NIST Webbook
tc	520.44 ± 0.40	K	NIST Webbook

tc	520.50	K	KDB
tc	520.50 ± 0.50	K	NIST Webbook
tf	149.30	K	KDB
tf	149.25	K	Aqueous Solubility Prediction Method
tt	149.37 ± 0.08	K	NIST Webbook
tt	149.37 ± 0.06	K	NIST Webbook
tt	149.41 ± 0.03	K	NIST Webbook
tt	148.10 ± 0.20	K	NIST Webbook
tt	149.43 ± 0.06	K	NIST Webbook
tt	149.42 ± 0.02	K	NIST Webbook
tt	149.38 ± 0.05	K	NIST Webbook
vc	0.416	m3/kmol	NIST Webbook
vc	0.416	m3/kmol	KDB
zc	0.2662660		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.45	J/mol×K	530.89	Joback Method
cpg	255.86	J/mol×K	501.80	Joback Method
cpg	194.59	J/mol×K	356.33	Joback Method
cpg	208.03	J/mol×K	385.42	Joback Method
cpg	220.86	J/mol×K	414.52	Joback Method
cpg	233.09	J/mol×K	443.61	Joback Method
cpg	244.75	J/mol×K	472.71	Joback Method
cpl	217.10	J/mol×K	294.10	NIST Webbook
cpl	221.12	J/mol×K	298.15	NIST Webbook
dvisc	0.0112423	Pa×s	171.07	Joback Method
dvisc	0.0038120	Pa×s	201.95	Joback Method
dvisc	0.0017220	Pa×s	232.82	Joback Method
dvisc	0.0009370	Pa×s	263.70	Joback Method
dvisc	0.0005792	Pa×s	294.58	Joback Method
dvisc	0.0003923	Pa×s	325.45	Joback Method
dvisc	0.0002842	Pa×s	356.33	Joback Method
hfust	5.82	kJ/mol	149.43	NIST Webbook
hfust	5.86	kJ/mol	148.10	NIST Webbook
hfust	5.86	kJ/mol	148.10	NIST Webbook
hfust	5.86	kJ/mol	148.10	NIST Webbook
hvapt	31.80 ± 0.10	kJ/mol	308.00	NIST Webbook

hvapt	30.50 ± 0.10	kJ/mol	330.00	NIST Webbook
hvapt	30.10 ± 0.10	kJ/mol	338.00	NIST Webbook
hvapt	29.40 ± 0.10	kJ/mol	348.00	NIST Webbook
hvapt	28.80 ± 0.10	kJ/mol	358.00	NIST Webbook
hvapt	28.10 ± 0.10	kJ/mol	368.00	NIST Webbook
hvapt	30.10	kJ/mol	418.00	NIST Webbook
hvapt	32.80	kJ/mol	319.00	NIST Webbook
hvapt	32.60	kJ/mol	320.50	NIST Webbook
hvapt	31.00 ± 0.10	kJ/mol	323.00	NIST Webbook
hvapt	31.40 ± 0.10	kJ/mol	315.00	NIST Webbook
hvapt	29.16	kJ/mol	352.40	KDB
hvapt	29.23	kJ/mol	352.40	NIST Webbook
hvapt	33.20	kJ/mol	315.50	NIST Webbook
rfi	1.37955		298.15	KDB
rhoI	674.00	kg/m3	293.00	KDB
sfust	39.58	J/mol×K	148.10	NIST Webbook
sfust	38.98	J/mol×K	149.43	NIST Webbook
srf	0.02	N/m	298.20	KDB
tcondl	0.10	W/m×K	297.02	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
tcondl	0.09	W/m×K	317.95	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
tcondl	0.09	W/m×K	336.91	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
tcondl	0.09	W/m×K	317.63	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)

tcondl	0.09	W/m×K	317.22	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.09	W/m×K	337.31	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.10	W/m×K	296.69	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.10	W/m×K	296.32	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.10	W/m×K	276.13	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.10	W/m×K	275.83	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.10	W/m×K	275.45	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)

tcondl	0.11	W/m×K	256.84	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.11	W/m×K	256.52	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.09	W/m×K	337.64	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.11	W/m×K	256.16	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	351.20	K	99.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41875e+01
Coeff. B	-3.04378e+03
Coeff. C	-3.42570e+01
Temperature range (K), min.	253.24
Temperature range (K), max.	377.18

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	6.63234e+01
Coeff. B	-5.95594e+03
Coeff. C	-7.76366e+00
Coeff. D	5.84993e-06
Temperature range (K), min.	149.34
Temperature range (K), max.	520.50

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=42
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C590352&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of KDBs: C_nH_{2n+2} (n = 6 to 8):	https://www.doi.org/10.1021/je020125e
KDBs:	https://www.thermo.com/files/research/kdb/mol/mol42.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rhof:	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
tbrp:	Boiling point at reduced pressure
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

Latest version available from:

<https://www.chemeo.com/cid/15-697-2/Pentane-2-2-dimethyl.pdf>

Generated by Cheméo on 2025-12-22 05:53:18.731957272 +0000 UTC m=+6130996.261997925.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.