

Pentane, 2,4-dimethyl-

Other names:	2,4-Dimethylpentane
Inchi:	InChI=1S/C7H16/c1-6(2)5-7(3)4/h6-7H,5H2,1-4H3
InchiKey:	BZHMBWZPUJHVEE-UHFFFAOYSA-N
Formula:	C7H16
SMILES:	CC(C)CC(C)C
Mol. weight [g/mol]:	100.20
CAS:	108-08-7

Physical Properties

Property code	Value	Unit	Source
af	0.3020		KDB
ap	351.950	K	KDB
chl	-4806.29 ± 0.84	kJ/mol	NIST Webbook
chl	-4802.00 ± 1.00	kJ/mol	NIST Webbook
dm	0.00	debye	KDB
gf	3.10	kJ/mol	KDB
hcg	4806.29	kJ/mol	KDB
hcn	4454.161	kJ/mol	KDB
hf	-202.10	kJ/mol	KDB
hf	-202.10 ± 0.96	kJ/mol	NIST Webbook
hf	-205.10	kJ/mol	NIST Webbook
hfl	-238.00 ± 1.00	kJ/mol	NIST Webbook
hfl	-235.00 ± 0.96	kJ/mol	NIST Webbook
hfus	6.84	kJ/mol	Joback Method
hvap	33.02	kJ/mol	NIST Webbook
hvap	32.70 ± 0.10	kJ/mol	NIST Webbook
hvap	32.88	kJ/mol	NIST Webbook
hvap	32.90 ± 0.10	kJ/mol	NIST Webbook
log10ws	-4.26		Aqueous Solubility Prediction Method
log10ws	-4.26		Estimated Solubility Method
logp	2.688		Crippen Method
mcvol	109.490	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
pc	2776.30 ± 50.66	kPa	NIST Webbook
pc	2736.70 ± 40.53	kPa	NIST Webbook
pc	2740.00	kPa	KDB

pc	2740.00 ± 50.00	kPa	NIST Webbook
rhoc	240.48 ± 5.01	kg/m3	NIST Webbook
rhoc	240.48 ± 5.01	kg/m3	NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	632.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	628.90		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	632.00		NIST Webbook
rinpol	626.30		NIST Webbook
rinpol	630.30		NIST Webbook
rinpol	634.90		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	630.80		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	630.90		NIST Webbook
rinpol	630.70		NIST Webbook
rinpol	629.30		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	630.40		NIST Webbook
rinpol	630.50		NIST Webbook
rinpol	631.30		NIST Webbook
rinpol	629.80		NIST Webbook
rinpol	630.50		NIST Webbook
rinpol	629.30		NIST Webbook
rinpol	629.80		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	632.00		NIST Webbook
rinpol	633.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	630.20		NIST Webbook
rinpol	629.90		NIST Webbook
rinpol	630.40		NIST Webbook

rinpol	630.90	NIST Webbook
rinpol	631.50	NIST Webbook
rinpol	631.00	NIST Webbook
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rinpol	632.00	NIST Webbook
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rinpol	632.00	NIST Webbook
rinpol	633.00	NIST Webbook
rinpol	628.70	NIST Webbook
rinpol	629.00	NIST Webbook
rinpol	629.30	NIST Webbook
rinpol	629.60	NIST Webbook
rinpol	630.00	NIST Webbook
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rinpol	631.00	NIST Webbook
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rinpol	630.50	NIST Webbook
rinpol	631.20	NIST Webbook
rinpol	631.90	NIST Webbook
rinpol	632.60	NIST Webbook
rinpol	633.40	NIST Webbook
rinpol	634.20	NIST Webbook
rinpol	633.70	NIST Webbook
rinpol	633.10	NIST Webbook
rinpol	632.20	NIST Webbook
rinpol	631.50	NIST Webbook
rinpol	630.60	NIST Webbook
rinpol	629.60	NIST Webbook
rinpol	627.00	NIST Webbook
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rinpol	631.00	NIST Webbook

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rinpol	630.00	NIST Webbook
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rinpol	633.19	NIST Webbook
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rinpol	633.57	NIST Webbook
rinpol	632.42	NIST Webbook
rinpol	632.98	NIST Webbook
rinpol	631.00	NIST Webbook
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rinpol	630.00	NIST Webbook
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rinpol	621.00	NIST Webbook

rinpol	630.60		NIST Webbook
rinpol	633.00		NIST Webbook
rinpol	627.10		NIST Webbook
rinpol	620.63		NIST Webbook
rinpol	621.45		NIST Webbook
rinpol	621.20		NIST Webbook
rinpol	625.80		NIST Webbook
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rinpol	623.10		NIST Webbook
rinpol	623.73		NIST Webbook
rinpol	623.75		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	624.00		NIST Webbook
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rinpol	626.00		NIST Webbook
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rinpol	630.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	634.00		NIST Webbook
ripol	611.00		NIST Webbook
ripol	609.00		NIST Webbook
sg	396.73	J/mol×K	NIST Webbook
sl	291.60	J/mol×K	NIST Webbook
sl	303.17	J/mol×K	NIST Webbook
tb	353.64	K	KDB

tc	519.80	K	KDB
tc	519.80 ± 0.50	K	NIST Webbook
tc	520.25 ± 0.50	K	NIST Webbook
tc	521.70 ± 2.00	K	NIST Webbook
tc	519.73 ± 0.40	K	NIST Webbook
tf	153.20	K	KDB
tf	152.52	K	Aqueous Solubility Prediction Method
vc	0.418	m3/kmol	KDB
vc	0.418	m3/kmol	NIST Webbook
zc	0.2650050		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.84	J/mol×K	358.68	Joback Method
cpg	206.39	J/mol×K	387.25	Joback Method
cpg	218.48	J/mol×K	415.82	Joback Method
cpg	230.12	J/mol×K	444.39	Joback Method
cpg	241.33	J/mol×K	472.96	Joback Method
cpg	252.10	J/mol×K	501.53	Joback Method
cpg	262.46	J/mol×K	530.10	Joback Method
cpl	220.90	J/mol×K	294.40	NIST Webbook
cpl	224.22	J/mol×K	298.15	NIST Webbook
dvisc	0.0048239	Pa×s	175.32	Joback Method
dvisc	0.0017200	Pa×s	211.99	Joback Method
dvisc	0.0008313	Pa×s	248.66	Joback Method
dvisc	0.0233449	Pa×s	138.65	Joback Method
dvisc	0.0002290	Pa×s	358.68	Joback Method
dvisc	0.0003191	Pa×s	322.01	Joback Method
dvisc	0.0004843	Pa×s	285.34	Joback Method
hfust	6.69	kJ/mol	152.50	NIST Webbook
hfust	6.85	kJ/mol	154.00	NIST Webbook
hfust	6.84	kJ/mol	153.97	NIST Webbook
hvapt	31.50 ± 0.10	kJ/mol	323.00	NIST Webbook
hvapt	31.00 ± 0.10	kJ/mol	330.00	NIST Webbook
hvapt	33.20	kJ/mol	320.50	NIST Webbook
hvapt	29.55	kJ/mol	353.70	NIST Webbook
hvapt	29.50	kJ/mol	353.80	KDB
hvapt	31.90 ± 0.10	kJ/mol	315.00	NIST Webbook

hvapt	30.00 ± 0.10	kJ/mol	348.00	NIST Webbook
hvapt	33.30	kJ/mol	319.50	NIST Webbook
hvapt	32.30 ± 0.10	kJ/mol	308.00	NIST Webbook
hvapt	30.60 ± 0.10	kJ/mol	338.00	NIST Webbook
rfi	1.37882		298.15	KDB
rhoI	673.00	kg/m3	293.00	KDB
sfust	44.46	J/mol×K	153.97	NIST Webbook
sfust	43.90	J/mol×K	152.50	NIST Webbook
srf	0.02	N/m	298.20	KDB
tcondI	0.11	W/m×K	277.04	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
tcondI	0.11	W/m×K	256.99	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
tcondI	0.11	W/m×K	257.30	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
tcondI	0.11	W/m×K	276.30	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
tcondI	0.11	W/m×K	276.69	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
tcondI	0.11	W/m×K	256.59	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)

tcondl	0.10	W/m×K	296.19	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
tcondl	0.10	W/m×K	296.63	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
tcondl	0.10	W/m×K	296.97	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
tcondl	0.10	W/m×K	316.55	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
tcondl	0.10	W/m×K	317.01	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)
tcondl	0.10	W/m×K	317.37	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	333.96	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	334.43	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	334.81	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41563e+01
Coeff. B	-3.00079e+03
Coeff. C	-3.90250e+01
Temperature range (K), min.	255.40
Temperature range (K), max.	378.30

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	8.06735e+01
Coeff. B	-6.55171e+03
Coeff. C	-9.98037e+00
Coeff. D	8.33917e-06
Temperature range (K), min.	153.91
Temperature range (K), max.	519.79

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
283.15	95.00	681.7
283.15	4961.00	686.3
283.15	9969.00	690.9
283.15	14980.00	695.1
283.15	19985.00	699.1
283.15	25039.00	702.9
283.15	30016.00	706.5
283.15	35089.00	710.0
283.15	40016.00	713.3
283.15	45012.00	716.4
283.15	49972.00	719.5
283.15	54980.00	722.4
283.15	59931.00	725.3
283.15	65047.00	728.1
288.15	127.00	677.3
288.15	4984.00	682.2
288.15	9987.00	686.8
288.15	14976.00	691.2
288.15	19996.00	695.3
288.15	24895.00	699.2
288.15	30002.00	703.0
288.15	34983.00	706.5
288.15	40000.00	709.9
288.15	44974.00	713.1
288.15	49950.00	716.2
288.15	55010.00	719.3
288.15	60065.00	722.2
288.15	64958.00	725.0
293.15	83.00	672.8
293.15	4982.00	677.9
293.15	9969.00	682.7
293.15	15059.00	687.3
293.15	19914.00	691.5
293.15	25056.00	695.6
293.15	29936.00	699.3
293.15	34976.00	703.0
293.15	39994.00	706.4
293.15	44992.00	709.8
293.15	50030.00	713.0

293.15	54953.00	716.0
293.15	59933.00	719.0
293.15	65045.00	721.9
298.15	92.00	668.3
298.15	4941.00	673.6
298.15	9982.00	678.6
298.15	14991.00	683.3
298.15	19963.00	687.6
298.15	25048.00	691.8
298.15	29972.00	695.7
298.15	34945.00	699.4
298.15	39958.00	702.9
298.15	45007.00	706.4
298.15	49963.00	709.6
298.15	55008.00	712.8
298.15	60003.00	715.8
298.15	65017.00	718.8
303.15	72.00	663.8
303.15	4969.00	669.3
303.15	9974.00	674.5
303.15	14963.00	679.3
303.15	19981.00	683.9
303.15	25047.00	688.2
303.15	29954.00	692.1
303.15	34987.00	695.9
303.15	39964.00	699.6
303.15	45006.00	703.1
303.15	49991.00	706.4
303.15	55060.00	709.7
303.15	59991.00	712.8
303.15	65054.00	715.8
308.15	100.00	659.4
308.15	4987.00	665.1
308.15	9965.00	670.4
308.15	15040.00	675.5
308.15	19960.00	680.1
308.15	24964.00	684.4
308.15	30076.00	688.7
308.15	34985.00	692.5
308.15	39972.00	696.2
308.15	44972.00	699.8
308.15	49955.00	703.2
308.15	54996.00	706.5
308.15	60063.00	709.7

308.15	65021.00	712.7
313.15	108.00	654.9
313.15	5004.00	660.8
313.15	10013.00	666.4
313.15	15049.00	671.6
313.15	19963.00	676.3
313.15	25062.00	680.9
313.15	29960.00	685.0
313.15	34942.00	689.0
313.15	40039.00	692.9
313.15	45017.00	696.6
313.15	50065.00	700.1
313.15	54977.00	703.4
313.15	59923.00	706.6
313.15	64996.00	709.7
318.15	110.00	650.2
318.15	5061.00	656.5
318.15	9957.00	662.2
318.15	15002.00	667.6
318.15	19980.00	672.5
318.15	25013.00	677.1
318.15	30045.00	681.5
318.15	34965.00	685.6
318.15	39938.00	689.5
318.15	44971.00	693.2
318.15	49989.00	696.8
318.15	55009.00	700.2
318.15	59952.00	703.5
318.15	65056.00	706.7
323.15	121.00	645.6
323.15	5001.00	652.1
323.15	10007.00	658.1
323.15	15037.00	663.6
323.15	19969.00	668.7
323.15	25018.00	673.5
323.15	29938.00	677.9
323.15	35006.00	682.2
323.15	39965.00	686.1
323.15	45012.00	690.0
323.15	49970.00	693.6
323.15	54953.00	697.1
323.15	59965.00	700.4
323.15	65022.00	703.7
328.15	98.00	641.0

328.15	5010.00	647.8
328.15	9934.00	653.9
328.15	14950.00	659.6
328.15	19968.00	664.9
328.15	25011.00	669.8
328.15	30040.00	674.5
328.15	34952.00	678.7
328.15	39959.00	682.8
328.15	45017.00	686.8
328.15	49935.00	690.4
328.15	54941.00	694.0
328.15	59962.00	697.4
328.15	65006.00	700.8
333.15	92.00	636.3
333.15	4968.00	643.3
333.15	9977.00	649.8
333.15	15014.00	655.7
333.15	19986.00	661.1
333.15	25001.00	666.2
333.15	29959.00	670.9
333.15	34922.00	675.3
333.15	39972.00	679.5
333.15	45064.00	683.6
333.15	50006.00	687.3
333.15	54975.00	691.0
333.15	59984.00	694.5
333.15	64995.00	697.8
338.15	107.00	631.7
338.15	5007.00	639.1
338.15	9978.00	645.7
338.15	14968.00	651.8
338.15	19968.00	657.4
338.15	25042.00	662.7
338.15	30018.00	667.5
338.15	35052.00	672.1
338.15	39990.00	676.3
338.15	45087.00	680.5
338.15	49968.00	684.3
338.15	55044.00	688.1
338.15	60031.00	691.6
338.15	64997.00	695.0
343.15	98.00	626.8
343.15	4944.00	634.4
343.15	10008.00	641.5

343.15	14958.00	647.7
343.15	19959.00	653.5
343.15	25045.00	658.9
343.15	30012.00	663.9
343.15	34980.00	668.5
343.15	40024.00	672.9
343.15	44956.00	677.1
343.15	50037.00	681.1
343.15	55010.00	684.9
343.15	59979.00	688.5
343.15	65088.00	692.1
348.15	103.00	622.0
348.15	4998.00	630.0
348.15	9948.00	637.2
348.15	15016.00	643.8
348.15	19991.00	649.7
348.15	25051.00	655.3
348.15	29994.00	660.3
348.15	34970.00	665.1
348.15	39979.00	669.6
348.15	45063.00	673.9
348.15	50024.00	678.0
348.15	54974.00	681.8
348.15	59994.00	685.5
353.15	1014.00	618.8
353.15	5010.00	625.6
353.15	9950.00	633.0
353.15	15037.00	639.9
353.15	19996.00	646.0
353.15	25024.00	651.7
353.15	29983.00	656.9
353.15	34950.00	661.8
353.15	40060.00	666.5
353.15	45017.00	670.8
353.15	49987.00	674.9
353.15	54976.00	678.9
353.15	59989.00	682.7
358.15	5026.00	621.0
358.15	9954.00	628.7
358.15	15017.00	635.8
358.15	19926.00	642.0
358.15	25014.00	647.9
358.15	30045.00	653.4
358.15	35004.00	658.3

358.15	40013.00	663.1
358.15	44988.00	667.5
358.15	49996.00	671.7
358.15	55037.00	675.8
358.15	60020.00	679.6
358.15	65016.00	683.3
363.15	4947.00	616.2
363.15	10031.00	624.5
363.15	15019.00	631.7
363.15	19970.00	638.2
363.15	25122.00	644.3
363.15	30059.00	649.8
363.15	35064.00	654.9
363.15	40055.00	659.8
363.15	45078.00	664.3
363.15	49933.00	668.5
363.15	54989.00	672.7
363.15	59992.00	676.6
363.15	65058.00	680.3

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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
nfpaf:	NFPA Fire Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhoc:	Critical density
rhof:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	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
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter

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