

Pentane, 2,3,4-trimethyl-

Other names:	(CH3)2CHCH(CH3)CH(CH3)2 2,3,4-Trimethylpentane
Inchi:	InChI=1S/C8H18/c1-6(2)8(5)7(3)4/h6-8H,1-5H3
InchiKey:	RLPGDEORIPLBNF-UHFFFAOYSA-N
Formula:	C8H18
SMILES:	CC(C)C(C)C(C)C
Mol. weight [g/mol]:	114.23
CAS:	565-75-3

Physical Properties

Property code	Value	Unit	Source
af	0.3150		KDB
ap	341.450	K	KDB
chl	-5465.50 ± 1.60	kJ/mol	NIST Webbook
gf	18.92	kJ/mol	KDB
hcg	5465.48	kJ/mol	KDB
hcn	5069.335	kJ/mol	KDB
hf	-217.60	kJ/mol	KDB
hf	-217.40 ± 1.70	kJ/mol	NIST Webbook
hfl	-255.20 ± 1.70	kJ/mol	NIST Webbook
hfus	5.91	kJ/mol	Joback Method
hvap	37.82	kJ/mol	NIST Webbook
hvap	37.70	kJ/mol	NIST Webbook
hvap	37.70 ± 0.10	kJ/mol	NIST Webbook
hvap	37.70 ± 0.10	kJ/mol	NIST Webbook
hvap	37.70	kJ/mol	NIST Webbook
log10ws	-4.80		Estimated Solubility Method
log10ws	-4.80		Aqueous Solubility Prediction Method
logp	2.934		Crippen Method
mccvol	123.580	ml/mol	McGowan Method
pc	2729.80 ± 40.53	kPa	NIST Webbook
pc	2730.00 ± 40.00	kPa	NIST Webbook
pc	2730.00	kPa	KDB
rhoc	247.88 ± 4.57	kg/m3	NIST Webbook
rhoc	247.88 ± 4.57	kg/m3	NIST Webbook
rinpol	765.10		NIST Webbook

rinpol	749.00	NIST Webbook
rinpol	764.20	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	752.00	NIST Webbook
rinpol	748.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	754.00	NIST Webbook
rinpol	751.60	NIST Webbook
rinpol	755.05	NIST Webbook
rinpol	748.40	NIST Webbook
rinpol	749.80	NIST Webbook
rinpol	751.20	NIST Webbook
rinpol	752.70	NIST Webbook
rinpol	747.00	NIST Webbook
rinpol	748.00	NIST Webbook
rinpol	749.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	752.00	NIST Webbook
rinpol	754.00	NIST Webbook
rinpol	748.30	NIST Webbook
rinpol	749.60	NIST Webbook
rinpol	751.00	NIST Webbook
rinpol	752.50	NIST Webbook
rinpol	754.00	NIST Webbook
rinpol	755.60	NIST Webbook
rinpol	751.90	NIST Webbook
rinpol	751.90	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	748.20	NIST Webbook
rinpol	749.70	NIST Webbook
rinpol	751.30	NIST Webbook
rinpol	752.90	NIST Webbook
rinpol	754.60	NIST Webbook
rinpol	756.40	NIST Webbook
rinpol	747.70	NIST Webbook
rinpol	748.30	NIST Webbook
rinpol	749.30	NIST Webbook
rinpol	750.10	NIST Webbook
rinpol	751.10	NIST Webbook
rinpol	752.00	NIST Webbook
rinpol	755.00	NIST Webbook

rinpol	756.00	NIST Webbook
rinpol	754.00	NIST Webbook
rinpol	754.00	NIST Webbook
rinpol	754.00	NIST Webbook
rinpol	755.50	NIST Webbook
rinpol	752.00	NIST Webbook
rinpol	755.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	752.00	NIST Webbook
rinpol	752.00	NIST Webbook
rinpol	748.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	771.30	NIST Webbook
rinpol	752.00	NIST Webbook
rinpol	754.00	NIST Webbook
rinpol	752.50	NIST Webbook
rinpol	754.00	NIST Webbook
rinpol	748.00	NIST Webbook
rinpol	758.00	NIST Webbook
rinpol	751.00	NIST Webbook
rinpol	749.00	NIST Webbook
rinpol	752.00	NIST Webbook
rinpol	755.00	NIST Webbook
rinpol	757.00	NIST Webbook
rinpol	750.50	NIST Webbook
rinpol	753.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	752.00	NIST Webbook
rinpol	756.00	NIST Webbook
rinpol	751.00	NIST Webbook
rinpol	754.00	NIST Webbook
rinpol	756.00	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	753.00	NIST Webbook
rinpol	746.70	NIST Webbook
rinpol	752.00	NIST Webbook
rinpol	759.00	NIST Webbook
rinpol	743.63	NIST Webbook
rinpol	747.60	NIST Webbook
rinpol	744.80	NIST Webbook
rinpol	748.00	NIST Webbook
rinpol	745.00	NIST Webbook
rinpol	743.00	NIST Webbook

rinpol	757.70		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	752.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	752.00		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	746.00		NIST Webbook
rinpol	752.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	757.00		NIST Webbook
rinpol	752.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	746.00		NIST Webbook
rinpol	746.00		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	761.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	761.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	765.60		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	750.20		NIST Webbook
rinpol	747.10		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	759.00		NIST Webbook
sg	427.20 ± 1.30	J/mol×K	NIST Webbook
sl	329.32	J/mol×K	NIST Webbook
tb	386.60	K	KDB
tc	566.40	K	KDB
tc	566.40 ± 0.50	K	NIST Webbook
tc	566.30	K	NIST Webbook

tc	566.34 ± 0.50	K	NIST Webbook
tf	163.90	K	KDB
tf	163.75	K	Aqueous Solubility Prediction Method
tt	163.63 ± 0.12	K	NIST Webbook
vc	0.460	m3/kmol	NIST Webbook
vc	0.460	m3/kmol	KDB
zc	0.2666620		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.96 ± 0.61	J/mol×K	523.15	NIST Webbook
cpg	246.46 ± 0.49	J/mol×K	398.15	NIST Webbook
cpg	248.11	J/mol×K	402.80	NIST Webbook
cpg	251.50 ± 2.50	J/mol×K	417.00	NIST Webbook
cpg	258.52 ± 0.52	J/mol×K	423.15	NIST Webbook
cpg	271.05 ± 0.54	J/mol×K	448.15	NIST Webbook
cpg	276.98	J/mol×K	463.60	NIST Webbook
cpg	283.03 ± 0.57	J/mol×K	473.15	NIST Webbook
cpg	293.98 ± 0.59	J/mol×K	498.15	NIST Webbook
cpg	303.34	J/mol×K	521.60	NIST Webbook
cpg	233.50 ± 0.47	J/mol×K	373.15	NIST Webbook
cpl	247.32	J/mol×K	298.15	NIST Webbook
cpl	246.23	J/mol×K	293.79	NIST Webbook
dvisc	0.0003235	Pa×s	340.09	Joback Method
dvisc	0.0005201	Pa×s	299.05	Joback Method
dvisc	0.0009727	Pa×s	258.02	Joback Method
dvisc	0.0023051	Pa×s	216.99	Joback Method
dvisc	0.0081685	Pa×s	175.95	Joback Method
dvisc	0.0624902	Pa×s	134.92	Joback Method
dvisc	0.0002228	Pa×s	381.12	Joback Method
hfust	9.27	kJ/mol	163.60	NIST Webbook
hfust	9.27	kJ/mol	163.60	NIST Webbook
hfust	9.27	kJ/mol	163.63	NIST Webbook
hvapt	39.80	kJ/mol	250.50	NIST Webbook
hvapt	32.73	kJ/mol	386.60	KDB
hvapt	37.70	kJ/mol	344.00	NIST Webbook
hvapt	32.36	kJ/mol	386.60	NIST Webbook
hvapt	36.70	kJ/mol	349.00	NIST Webbook
hvapt	41.30	kJ/mol	324.50	NIST Webbook

hvapt	39.10	kJ/mol	256.00	NIST Webbook	
rfi	1.40198		298.15	KDB	
rhoI	719.00	kg/m3	293.00	KDB	
sfust	56.64	J/mol×K	163.63	NIST Webbook	
srf	0.02	N/m	298.20	KDB	
tcondI	0.10	W/m×K	297.58	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)	
tcondI	0.10	W/m×K	316.03	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)	
tcondI	0.10	W/m×K	332.39	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)	
tcondI	0.10	W/m×K	332.13	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)	
tcondI	0.10	W/m×K	331.87	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)	
tcondI	0.10	W/m×K	297.33	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C _n H _{2n+2} (n = 6 to 8)	
tcondI	0.10	W/m×K	315.77	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	315.53	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.10	W/m×K	297.84	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.11	W/m×K	278.19	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.11	W/m×K	277.95	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.11	W/m×K	259.54	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.11	W/m×K	259.29	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)
tcondl	0.11	W/m×K	259.06	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: CnH2n+2 (n = 6 to 8)

tcondl	0.11	W/m×K	278.44	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(Pvp) = A + B/(T + C)
Coeff. A	1.42673e+01
Coeff. B	-3.34524e+03
Coeff. C	-3.99270e+01
Temperature range (K), min.	279.22
Temperature range (K), max.	413.45

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.53988e+01
Coeff. B	-6.92178e+03
Coeff. C	-9.02988e+00
Coeff. D	6.13464e-06
Temperature range (K), min.	163.95
Temperature range (K), max.	566.30

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
283.15	130.00	728.3
283.15	4973.00	732.2

283.15	9993.00	736.0
283.15	14965.00	739.6
283.15	20000.00	743.0
283.15	25003.00	746.3
283.15	29990.00	749.5
283.15	35009.00	752.5
283.15	39961.00	755.4
283.15	45014.00	758.3
283.15	49986.00	761.0
283.15	54944.00	763.6
283.15	60030.00	766.3
283.15	65014.00	768.8
288.15	102.00	724.3
288.15	5015.00	728.4
288.15	9991.00	732.3
288.15	14975.00	736.0
288.15	20038.00	739.6
288.15	25021.00	743.0
288.15	29929.00	746.1
288.15	35037.00	749.3
288.15	40039.00	752.3
288.15	44998.00	755.2
288.15	49927.00	757.9
288.15	54967.00	760.6
288.15	59925.00	763.2
288.15	65032.00	765.9
293.15	111.00	720.4
293.15	5021.00	724.6
293.15	9998.00	728.6
293.15	14997.00	732.4
293.15	19997.00	736.1
293.15	25022.00	739.6
293.15	29930.00	742.8
293.15	34968.00	746.0
293.15	39974.00	749.1
293.15	45009.00	752.0
293.15	49965.00	754.9
293.15	54987.00	757.6
293.15	59945.00	760.3
293.15	65000.00	762.9
298.15	105.00	716.2
298.15	5072.00	720.6
298.15	9964.00	724.7
298.15	15013.00	728.7

298.15	20054.00	732.5
298.15	25008.00	736.0
298.15	29968.00	739.4
298.15	34937.00	742.6
298.15	40018.00	745.8
298.15	45064.00	748.8
298.15	50010.00	751.7
298.15	55015.00	754.5
298.15	59955.00	757.2
298.15	65024.00	759.9
303.15	100.00	712.0
303.15	4934.00	716.5
303.15	10038.00	720.9
303.15	14973.00	724.9
303.15	19957.00	728.7
303.15	25002.00	732.4
303.15	29980.00	735.9
303.15	34972.00	739.3
303.15	39972.00	742.5
303.15	44990.00	745.6
303.15	49984.00	748.5
303.15	54948.00	751.4
303.15	59951.00	754.2
303.15	65040.00	756.9
308.15	92.00	707.8
308.15	5051.00	712.5
308.15	9961.00	716.8
308.15	14959.00	721.0
308.15	20027.00	725.0
308.15	25025.00	728.8
308.15	29996.00	732.4
308.15	34959.00	735.7
308.15	40017.00	739.1
308.15	45023.00	742.2
308.15	49965.00	745.2
308.15	54977.00	748.2
308.15	60020.00	751.0
308.15	64995.00	753.8
313.15	99.00	703.6
313.15	4997.00	708.5
313.15	9998.00	713.1
313.15	15010.00	717.4
313.15	19994.00	721.4
313.15	25007.00	725.3

313.15	29995.00	729.0
313.15	35008.00	732.4
313.15	39993.00	735.8
313.15	45005.00	739.0
313.15	49990.00	742.1
313.15	55003.00	745.1
313.15	59996.00	748.0
313.15	64993.00	750.8
318.15	104.00	699.5
318.15	4961.00	704.4
318.15	10003.00	709.2
318.15	15026.00	713.7
318.15	19937.00	717.8
318.15	25012.00	721.8
318.15	29990.00	725.5
318.15	34991.00	729.1
318.15	39976.00	732.5
318.15	45028.00	735.8
318.15	49973.00	739.0
318.15	54916.00	742.0
318.15	59988.00	744.9
318.15	65015.00	747.8
323.15	111.00	695.4
323.15	5025.00	700.6
323.15	10013.00	705.5
323.15	14973.00	710.0
323.15	20028.00	714.4
323.15	25014.00	718.4
323.15	29976.00	722.2
323.15	34994.00	725.9
323.15	39992.00	729.4
323.15	45046.00	732.8
323.15	49980.00	736.0
323.15	54968.00	739.1
323.15	59988.00	742.1
323.15	65068.00	745.0
328.15	94.00	691.3
328.15	4971.00	696.6
328.15	9997.00	701.7
328.15	14959.00	706.4
328.15	19969.00	710.9
328.15	25055.00	715.1
328.15	29960.00	719.0
328.15	34966.00	722.7

328.15	40013.00	726.3
328.15	45034.00	729.8
328.15	50015.00	733.1
328.15	54973.00	736.2
328.15	59955.00	739.2
328.15	64992.00	742.2
333.15	95.00	687.1
333.15	4934.00	692.6
333.15	9973.00	697.9
333.15	14973.00	702.8
333.15	19993.00	707.4
333.15	24959.00	711.6
333.15	29952.00	715.7
333.15	34974.00	719.5
333.15	39961.00	723.2
333.15	44999.00	726.7
333.15	49992.00	730.1
333.15	54798.00	733.2
333.15	59952.00	736.4
333.15	65050.00	739.5
338.15	115.00	683.1
338.15	4978.00	688.9
338.15	9970.00	694.3
338.15	14966.00	699.3
338.15	19960.00	703.9
338.15	24994.00	708.4
338.15	30030.00	712.5
338.15	34973.00	716.3
338.15	39979.00	720.0
338.15	45024.00	723.6
338.15	50019.00	727.1
338.15	54928.00	730.3
338.15	59953.00	733.5
338.15	64998.00	736.6
343.15	109.00	678.8
343.15	5084.00	684.9
343.15	9963.00	690.4
343.15	15039.00	695.6
343.15	20010.00	700.4
343.15	24998.00	704.9
343.15	30054.00	709.2
343.15	35048.00	713.2
343.15	40023.00	717.0
343.15	44967.00	720.6

343.15	50023.00	724.2
343.15	54967.00	727.5
343.15	59995.00	730.7
343.15	64954.00	733.8
348.15	112.00	674.5
348.15	5011.00	680.8
348.15	10066.00	686.6
348.15	14992.00	691.9
348.15	19955.00	696.8
348.15	25042.00	701.5
348.15	29986.00	705.8
348.15	35004.00	709.9
348.15	40002.00	713.9
348.15	44996.00	717.6
348.15	49994.00	721.1
348.15	54995.00	724.6
348.15	60005.00	727.9
348.15	65009.00	731.0
353.15	109.00	670.1
353.15	4963.00	676.6
353.15	9919.00	682.5
353.15	15039.00	688.2
353.15	19995.00	693.2
353.15	24983.00	698.0
353.15	29960.00	702.4
353.15	34985.00	706.7
353.15	39983.00	710.7
353.15	45037.00	714.5
353.15	49989.00	718.1
353.15	54953.00	721.6
353.15	59909.00	724.9
353.15	65052.00	728.2
358.15	118.00	665.9
358.15	4955.00	672.5
358.15	9916.00	678.7
358.15	15035.00	684.5
358.15	19946.00	689.6
358.15	25037.00	694.6
358.15	29963.00	699.2
358.15	35027.00	703.4
358.15	40010.00	707.5
358.15	44955.00	711.4
358.15	50023.00	715.1
358.15	54980.00	718.7

358.15	59952.00	722.0
358.15	65021.00	725.4
363.15	101.00	661.3
363.15	4941.00	668.3
363.15	9928.00	674.7
363.15	15005.00	680.6
363.15	19958.00	686.0
363.15	24923.00	691.0
363.15	29983.00	695.8
363.15	34922.00	700.1
363.15	39992.00	704.4
363.15	45038.00	708.4
363.15	49985.00	712.2
363.15	54981.00	715.8
363.15	59985.00	719.3
363.15	65038.00	722.6

Reference <https://www.doi.org/10.1021/acs.jced.9b00846>

Sources

KDB:	https://www.thermo.com/files/research/kdb/mol/mol62.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=62
P-r-T Data and Derivative Properties of 3-Methylpentane, 2,4-Dimethylpentane, and 2,3,4-Trimethylpentane from 283.15 to 363.15 K at Pressures up to 65 MPa: Crippen Method:	https://www.doi.org/10.1021/acs.jced.9b00846
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C565753&Units=SI
Infinite dilution activity coefficients, specific retention volumes and aqueous solubility prediction Method: Joback Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solvation energy method:	https://www.doi.org/10.1016/j.fluid.2006.07.015
Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C ₁₂ H ₂₆ (n-Heptacosane):	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
The Yaws Handbook of Vapor Pressure:	https://en.wikipedia.org/wiki/Joback_method
	https://www.doi.org/10.1021/je020125e
	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

Latest version available from:

<https://www.chemeo.com/cid/54-615-9/Pentane-2-3-4-trimethyl.pdf>

Generated by Cheméo on 2025-12-23 01:47:27.961198966 +0000 UTC m=+6202645.491239631.

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