

# Butane, 2,2,3-trimethyl-

<b>Other names:</b>	2,2,3-TRIMETHYLBUTANE 2,3,3-trimethylbutane TRIPTAN TRIPTANE pentamethylethane
<b>Inchi:</b>	InChI=1S/C7H16/c1-6(2)7(3,4)5/h6H,1-5H3
<b>InchiKey:</b>	ZISSAWUMDACLOM-UHFFFAOYSA-N
<b>Formula:</b>	C7H16
<b>SMILES:</b>	CC(C)C(C)(C)C
<b>Mol. weight [g/mol]:</b>	100.20
<b>CAS:</b>	464-06-2

## Physical Properties

Property code	Value	Unit	Source
af	0.2500		KDB
ap	345.350	K	KDB
chl	-4803.00 ± 1.00	kJ/mol	NIST Webbook
chl	-4804.40 ± 1.00	kJ/mol	NIST Webbook
chl	-4803.99 ± 0.50	kJ/mol	NIST Webbook
dm	0.00	debye	KDB
gf	4.27	kJ/mol	KDB
hcg	4804.36	kJ/mol	KDB
hcn	4452.236	kJ/mol	KDB
hf	-204.80 ± 1.10	kJ/mol	NIST Webbook
hf	-205.90	kJ/mol	NIST Webbook
hf	-204.90	kJ/mol	KDB
hfl	-236.90 ± 1.10	kJ/mol	NIST Webbook
hfl	-238.00 ± 1.00	kJ/mol	NIST Webbook
hfus	2.95	kJ/mol	Joback Method
hvap	32.00	kJ/mol	NIST Webbook
hvap	32.19	kJ/mol	NIST Webbook
hvap	32.04	kJ/mol	NIST Webbook
log10ws	-4.36		Aqueous Solubility Prediction Method
log10ws	-4.36		Estimated Solubility Method
logp	2.688		Crippen Method

mcvol	109.490	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
pc	2950.00	kPa	KDB
pc	2950.00 ± 50.00	kPa	NIST Webbook
pc	2953.20 ± 40.53	kPa	NIST Webbook
pc	3014.42 ± 50.66	kPa	NIST Webbook
rhoc	251.51 ± 5.01	kg/m3	NIST Webbook
rhoc	251.51 ± 5.01	kg/m3	NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	635.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	637.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	635.00		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	631.53		NIST Webbook
rinpol	630.41		NIST Webbook
rinpol	628.44		NIST Webbook
rinpol	631.28		NIST Webbook
rinpol	630.06		NIST Webbook
rinpol	627.97		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	628.62		NIST Webbook
rinpol	628.59		NIST Webbook
rinpol	632.00		NIST Webbook
rinpol	628.10		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	646.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	624.70		NIST Webbook
rinpol	637.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	633.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	628.00		NIST Webbook

rinpol	630.00	NIST Webbook
rinpol	627.00	NIST Webbook
rinpol	632.00	NIST Webbook
rinpol	631.40	NIST Webbook
rinpol	630.30	NIST Webbook
rinpol	628.00	NIST Webbook
rinpol	638.00	NIST Webbook
rinpol	651.00	NIST Webbook
rinpol	632.40	NIST Webbook
rinpol	628.10	NIST Webbook
rinpol	630.06	NIST Webbook
rinpol	628.00	NIST Webbook
rinpol	634.00	NIST Webbook
rinpol	634.81	NIST Webbook
rinpol	626.28	NIST Webbook
rinpol	632.40	NIST Webbook
rinpol	639.00	NIST Webbook
rinpol	634.81	NIST Webbook
rinpol	635.00	NIST Webbook
rinpol	652.00	NIST Webbook
rinpol	641.00	NIST Webbook
rinpol	630.00	NIST Webbook
rinpol	643.30	NIST Webbook
rinpol	638.00	NIST Webbook
rinpol	630.30	NIST Webbook
rinpol	637.90	NIST Webbook
rinpol	636.00	NIST Webbook
rinpol	649.70	NIST Webbook
rinpol	652.00	NIST Webbook
rinpol	635.00	NIST Webbook
rinpol	638.00	NIST Webbook
rinpol	641.00	NIST Webbook
rinpol	639.30	NIST Webbook
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rinpol	639.10	NIST Webbook
rinpol	637.00	NIST Webbook
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rinpol	637.00	NIST Webbook
rinpol	632.00	NIST Webbook
rinpol	641.00	NIST Webbook
rinpol	642.00	NIST Webbook
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rinpol	645.00	NIST Webbook
rinpol	639.00	NIST Webbook
rinpol	641.00	NIST Webbook
rinpol	641.50	NIST Webbook
rinpol	640.00	NIST Webbook
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rinpol	646.10	NIST Webbook
rinpol	648.87	NIST Webbook
rinpol	650.77	NIST Webbook
rinpol	642.14	NIST Webbook
rinpol	644.23	NIST Webbook
rinpol	628.00	NIST Webbook
rinpol	636.00	NIST Webbook
rinpol	636.00	NIST Webbook
rinpol	638.00	NIST Webbook
rinpol	639.00	NIST Webbook
rinpol	640.20	NIST Webbook
rinpol	642.00	NIST Webbook
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rinpol	640.00	NIST Webbook

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rinpol	636.00		NIST Webbook
rinpol	637.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	631.00		NIST Webbook
sl	27.11	J/molxK	NIST Webbook
sl	292.25	J/molxK	NIST Webbook
tb	354.03 ± 0.02	K	NIST Webbook
tb	354.10	K	NIST Webbook
tb	354.00	K	NIST Webbook
tb	354.01	K	KDB
tb	353.95 ± 0.20	K	NIST Webbook
tb	354.15 ± 0.20	K	NIST Webbook
tb	354.00 ± 0.20	K	NIST Webbook
tb	353.90 ± 0.20	K	NIST Webbook
tb	353.90 ± 0.50	K	NIST Webbook
tb	354.05 ± 0.50	K	NIST Webbook
tb	354.20 ± 0.30	K	NIST Webbook
tb	354.15 ± 0.50	K	NIST Webbook
tb	354.00 ± 0.30	K	NIST Webbook
tb	354.15 ± 0.20	K	NIST Webbook
tb	354.15 ± 0.50	K	NIST Webbook
tb	354.11 ± 0.10	K	NIST Webbook
tb	354.15 ± 0.20	K	NIST Webbook
tb	354.15 ± 0.50	K	NIST Webbook
tb	354.02 ± 0.05	K	NIST Webbook
tb	354.02 ± 0.05	K	NIST Webbook
tb	354.03 ± 0.10	K	NIST Webbook
tb	354.06 ± 0.10	K	NIST Webbook
tb	353.85 ± 1.00	K	NIST Webbook
tb	354.05 ± 0.20	K	NIST Webbook
tb	353.75 ± 0.30	K	NIST Webbook
tb	353.95 ± 0.30	K	NIST Webbook
tb	354.20 ± 0.10	K	NIST Webbook
tb	354.03 ± 0.06	K	NIST Webbook
tb	353.05 ± 0.50	K	NIST Webbook
tb	354.20 ± 0.10	K	NIST Webbook
tb	354.05 ± 0.20	K	NIST Webbook
tb	354.05 ± 0.30	K	NIST Webbook
tb	354.00 ± 0.20	K	NIST Webbook
tb	354.15 ± 0.30	K	NIST Webbook
tb	354.05 ± 0.30	K	NIST Webbook
tb	354.05 ± 0.20	K	NIST Webbook

tb	354.05 ± 0.50	K	NIST Webbook
tb	354.03 ± 0.30	K	NIST Webbook
tc	531.10 ± 0.30	K	NIST Webbook
tc	531.45 ± 0.50	K	NIST Webbook
tc	531.11 ± 0.40	K	NIST Webbook
tc	531.10	K	KDB
tc	531.10	K	NIST Webbook
tf	248.00	K	KDB
tt	248.48 ± 0.05	K	NIST Webbook
tt	248.56 ± 0.07	K	NIST Webbook
tt	247.70 ± 0.20	K	NIST Webbook
tt	248.53 ± 0.05	K	NIST Webbook
tt	248.53 ± 0.03	K	NIST Webbook
vc	0.398	m <sup>3</sup> /kmol	KDB
vc	0.398	m <sup>3</sup> /kmol	NIST Webbook
zc	0.2658840		KDB
zra	0.27		KDB

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.28 ± 0.20	J/mol×K	369.20	NIST Webbook
cpg	178.82 ± 0.18	J/mol×K	328.80	NIST Webbook
cpg	188.66 ± 0.19	J/mol×K	348.85	NIST Webbook
cpg	239.99 ± 0.24	J/mol×K	461.80	NIST Webbook
cpg	228.20 ± 0.23	J/mol×K	434.30	NIST Webbook
cpg	213.05 ± 0.21	J/mol×K	400.40	NIST Webbook
cpl	213.51	J/mol×K	298.15	NIST Webbook
cpl	208.40	J/mol×K	293.90	NIST Webbook
dvisc	0.0060600	Paxs	189.37	Joback Method
dvisc	0.0006224	Paxs	289.28	Joback Method
dvisc	0.0247264	Paxs	156.07	Joback Method
dvisc	0.0022618	Paxs	222.68	Joback Method
dvisc	0.0010909	Paxs	255.98	Joback Method
dvisc	0.0003987	Paxs	322.59	Joback Method
dvisc	0.0002776	Paxs	355.89	Joback Method
hfust	2.38	kJ/mol	121.00	NIST Webbook
hfust	2.20	kJ/mol	247.70	NIST Webbook
hfust	2.20	kJ/mol	247.70	NIST Webbook
hvapt	32.30	kJ/mol	320.50	NIST Webbook
hvapt	29.90	kJ/mol	418.00	NIST Webbook

hvapt	28.95	kJ/mol	354.00	KDB
hvapt	28.90	kJ/mol	354.00	NIST Webbook
hvapt	31.20 ± 0.10	kJ/mol	314.00	NIST Webbook
hvapt	32.40	kJ/mol	319.50	NIST Webbook
hvapt	31.90	kJ/mol	337.00	NIST Webbook
rfi	1.38692		298.15	KDB
rhol	690.00	kg/m <sup>3</sup>	293.00	KDB
sfust	8.88	J/mol×K	247.70	NIST Webbook
sfust	19.64	J/mol×K	121.00	NIST Webbook
srf	0.02	N/m	298.20	KDB
tcondl	0.10	W/m×K	257.81	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C <sub>n</sub> H <sub>2n+2</sub> (n = 6 to 8)
tcondl	0.10	W/m×K	277.90	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C <sub>n</sub> H <sub>2n+2</sub> (n = 6 to 8)
tcondl	0.10	W/m×K	278.17	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C <sub>n</sub> H <sub>2n+2</sub> (n = 6 to 8)
tcondl	0.10	W/m×K	296.29	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C <sub>n</sub> H <sub>2n+2</sub> (n = 6 to 8)
tcondl	0.10	W/m×K	296.58	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C <sub>n</sub> H <sub>2n+2</sub> (n = 6 to 8)
tcondl	0.09	W/m×K	296.87	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C <sub>n</sub> H <sub>2n+2</sub> (n = 6 to 8)

tcondl	0.09	W/m×K	313.91	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C <sub>n</sub> H <sub>2n+2</sub> (n = 6 to 8)
tcondl	0.09	W/m×K	314.21	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C <sub>n</sub> H <sub>2n+2</sub> (n = 6 to 8)
tcondl	0.09	W/m×K	314.52	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C <sub>n</sub> H <sub>2n+2</sub> (n = 6 to 8)
tcondl	0.10	W/m×K	257.53	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C <sub>n</sub> H <sub>2n+2</sub> (n = 6 to 8)
tcondl	0.09	W/m×K	331.48	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C <sub>n</sub> H <sub>2n+2</sub> (n = 6 to 8)
tcondl	0.09	W/m×K	331.79	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C <sub>n</sub> H <sub>2n+2</sub> (n = 6 to 8)
tcondl	0.11	W/m×K	257.27	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C <sub>n</sub> H <sub>2n+2</sub> (n = 6 to 8)



tcondl	0.10	W/m×K	277.62	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C <sub>n</sub> H <sub>2n+2</sub> (n = 6 to 8)
tcondl	0.09	W/m×K	331.18	Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C <sub>n</sub> H <sub>2n+2</sub> (n = 6 to 8)

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.39980e+01
Coeff. B	-2.95941e+03
Coeff. C	-3.85160e+01
Temperature range (K), min.	248.57
Temperature range (K), max.	379.21

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	6.99528e+01
Coeff. B	-6.02823e+03
Coeff. C	-8.37831e+00
Coeff. D	6.93600e-06
Temperature range (K), min.	248.57
Temperature range (K), max.	531.17

## Sources

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Infinite dilution activity coefficients, specific retention volumes and estimated solubility method for hydrocarbons in C78H158 branched alkane solvent:</b>	<a href="https://www.doi.org/10.1016/j.fluid.2006.07.015">https://www.doi.org/10.1016/j.fluid.2006.07.015</a> <a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</a> <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C464062&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C464062&amp;Units=SI</a>
<b>KDB Vapor Pressure Data:</b>	<a href="https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=46">https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=46</a>
<b>KDB:</b>	<a href="https://www.thermo.com/files/research/kdb/mol/mol46.mol">https://www.thermo.com/files/research/kdb/mol/mol46.mol</a>
<b>Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of KDB Pure (KDB Pure Thermophysical Properties Databank):</b>	<a href="https://www.doi.org/10.1021/je020125e">https://www.doi.org/10.1021/je020125e</a> <a href="https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=46">https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=46</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>

## Legend

<b>af:</b>	Acentric Factor
<b>ap:</b>	Aniline Point
<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>cpl:</b>	Liquid phase heat capacity
<b>dm:</b>	Dipole Moment
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hcg:</b>	Heat of Combustion, Gross form
<b>hcn:</b>	Heat of Combustion, Net Form
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>nfpaf:</b>	NFPA Fire Rating
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rfi:</b>	Refractive Index
<b>rhoc:</b>	Critical density
<b>rhol:</b>	Liquid Density
<b>rinpol:</b>	Non-polar retention indices
<b>sfust:</b>	Entropy of fusion at a given temperature
<b>sl:</b>	Liquid phase molar entropy at standard conditions

<b>srf:</b>	Surface Tension
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tcondl:</b>	Liquid thermal conductivity
<b>tf:</b>	Normal melting (fusion) point
<b>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume
<b>zc:</b>	Critical Compressibility
<b>zra:</b>	Rackett Parameter

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