Butane, 2-methyl-

Other names:	1,1,2-Trimethylethane
	1,1-Dimethylpropane
	2-Methylbutane
	Ethyldimethylmethane
	Exxsol isopentane S
	Isoamylhydride
	Isopentane
	Methylbutane
	NSC 119476
	iso-C5H12
	iso-Pentane
Inchi:	InChI=1S/C5H12/c1-4-5(2)3/h5H,4H2,1-3H3
InchiKey:	QWTDNUCVQCZILF-UHFFFAOYSA-N
Formula:	C5H12
SMILES:	CCC(C)C
Mol. weight [g/mol]:	72.15
CAS:	78-78-4

Physical Properties

Property code	Value	Unit	Source
chg	-3528.60 ± 0.63	kJ/mol	NIST Webbook
chg	-3527.60 ± 3.50	kJ/mol	NIST Webbook
chg	-3528.40 ± 0.92	kJ/mol	NIST Webbook
chl	-3503.30 ± 0.75	kJ/mol	NIST Webbook
chl	-3504.40 ± 0.84	kJ/mol	NIST Webbook
gf	-11.22	kJ/mol	Joback Method
hf	-153.70 ± 0.59	kJ/mol	NIST Webbook
hf	-154.10 ± 0.96	kJ/mol	NIST Webbook
hf	-154.50 ± 0.84	kJ/mol	NIST Webbook
hfl	-179.30 ± 0.84	kJ/mol	NIST Webbook
hfl	-178.20 ± 0.88	kJ/mol	NIST Webbook
hfus	5.18	kJ/mol	Joback Method
hvap	24.80	kJ/mol	NIST Webbook
hvap	24.80 ± 0.10	kJ/mol	NIST Webbook
hvap	25.00	kJ/mol	NIST Webbook
hvap	25.22	kJ/mol	NIST Webbook
ie	10.32	eV	NIST Webbook

ie	10.50 ± 0.05	eV	NIST Webbook
ie	10.32	eV	NIST Webbook
ie	10.30 ± 0.10	eV	NIST Webbook
ie	10.22	eV	NIST Webbook
ie	10.18	eV	NIST Webbook
ie	10.32 ± 0.05	eV	NIST Webbook
ie	11.00 ± 0.10	eV	NIST Webbook
ie	10.94	eV	NIST Webbook
ie	10.21	eV	NIST Webbook
log10ws	-3.18		Estimated Solubility Method
log10ws	-3.18		Aqueous Solubility Prediction Method
logp	2.052		Crippen Method
mcvol	81.310	ml/mol	McGowan Method
pc	3381.00 ± 50.66	kPa	NIST Webbook
pc	3380.00 ± 50.00	kPa	NIST Webbook
pc	3270.00 ± 98.07	kPa	NIST Webbook
pc	3335.50 ± 66.70	kPa	NIST Webbook
pc	3410.60 ± 10.13	kPa	NIST Webbook
rhoc	234.27 ± 4.33	kg/m3	NIST Webbook
rhoc	235.93 ± 3.61	kg/m3	NIST Webbook
rhoc	235.93 ± 7.21	kg/m3	NIST Webbook
rhoc	235.93 ± 2.16	kg/m3	NIST Webbook
rhoc	234.27 ± 4.33	kg/m3	NIST Webbook
rinpol	475.00		NIST Webbook
rinpol	474.00		NIST Webbook
rinpol	476.00		NIST Webbook
rinpol	476.00		NIST Webbook
rinpol	465.00		NIST Webbook
rinpol	461.00		NIST Webbook
rinpol	477.50		NIST Webbook
rinpol	477.00		NIST Webbook
rinpol	464.90		NIST Webbook
rinpol	466.10		NIST Webbook
rinpol	465.35		NIST Webbook
rinpol	465.39		NIST Webbook
rinpol	475.00		NIST Webbook
rinpol	465.11		NIST Webbook
rinpol	465.18		NIST Webbook
rinpol	465.00		NIST Webbook
rinpol	466.00		NIST Webbook
rinpol	474.00		NIST Webbook
rinpol	475.00		NIST Webbook
rinpol	474.00		NIST Webbook

rinpol	475.00	NIST Webbook
rinpol	475.00	NIST Webbook
rinpol	473.00	NIST Webbook
rinpol	476.00	NIST Webbook
rinpol	480.00	NIST Webbook
rinpol	474.00	NIST Webbook
rinpol	465.00	NIST Webbook
rinpol	466.20	NIST Webbook
rinpol	464.00	NIST Webbook
rinpol	475.00	NIST Webbook
rinpol	475.00	NIST Webbook
rinpol	476.00	NIST Webbook
rinpol	475.00	NIST Webbook
rinpol	475.00	NIST Webbook
rinpol	475.00	NIST Webbook
rinpol	475.00	NIST Webbook
rinpol	477.00	NIST Webbook
rinpol	466.00	NIST Webbook
rinpol	472.00	NIST Webbook
rinpol	474.00	NIST Webbook
rinpol	467.00	NIST Webbook
rinpol	476.00	NIST Webbook
rinpol	476.00	NIST Webbook
rinpol	476.00	NIST Webbook
rinpol	476.00	NIST Webbook
rinpol	477.50	NIST Webbook
rinpol	464.00	NIST Webbook
rinpol	474.00	NIST Webbook
rinpol	474.00	NIST Webbook
rinpol	477.00	NIST Webbook
rinpol	478.00	NIST Webbook
rinpol	474.00	NIST Webbook
rinpol	474.00	NIST Webbook
rinpol	474.00	NIST Webbook
rinpol	474.00	NIST Webbook
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rinpol	476.00	NIST Webbook
rinpol	476.00	NIST Webbook
rinpol	475.00	NIST Webbook
rinpol	474.00	NIST Webbook
rinpol	476.00	NIST Webbook
rinpol	477.00	NIST Webbook
rinpol	472.00	NIST Webbook
rinpol	471.00	NIST Webbook

rinpol	471.00		NIST Webbook
rinpol	470.00		NIST Webbook
rinpol	470.00		NIST Webbook
rinpol	474.37		NIST Webbook
rinpol	476.00		NIST Webbook
rinpol	475.60		NIST Webbook
rinpol	475.00		NIST Webbook
rinpol	475.00		NIST Webbook
rinpol	475.40		NIST Webbook
rinpol	474.50		NIST Webbook
rinpol	474.90		NIST Webbook
rinpol	468.00		NIST Webbook
rinpol	474.90		NIST Webbook
rinpol	475.40		NIST Webbook
rinpol	475.80		NIST Webbook
rinpol	470.00		NIST Webbook
rinpol	470.00		NIST Webbook
rinpol	469.00		NIST Webbook
rinpol	474.20		NIST Webbook
rinpol	475.00		NIST Webbook
rinpol	467.00		NIST Webbook
rinpol	475.00		NIST Webbook
ripol	467.00		NIST Webbook
ripol	471.00		NIST Webbook
sl	260.41	J/mol×K	NIST Webbook
sl	261.04	J/mol×K	NIST Webbook
sl	254.40	J/mol×K	NIST Webbook
tb	301.15	K	Isobaric vapor-liquid equilibrium for four binary systems of thiophene
tb	301.15	K	Isobaric vapor-liquid equilibrium for four binary systems of 3-methylthiophene
tc	479.98	K	Joback Method
tf	113.23	K	Aqueous Solubility Prediction Method
tt	112.60 ± 0.30	K	NIST Webbook
tt	113.39 ± 0.05	K	NIST Webbook
tt	113.37 ± 0.02	K	NIST Webbook
vc	0.306	m3/kmol	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.62 ± 0.54	J/mol×K	487.05	NIST Webbook
cpg	153.64 ± 0.46	J/mol×K	402.30	NIST Webbook
cpg	168.36 ± 0.51	J/mol×K	449.20	NIST Webbook
cpg	125.31 ± 0.37	J/mol×K	317.20	NIST Webbook
cpg	139.12 ± 0.42	J/mol×K	358.15	NIST Webbook
cpl	164.85	J/mol×K	298.15	NIST Webbook
cpl	164.50	J/mol×K	298.30	NIST Webbook
cpl	169.41	J/mol×K	290.00	NIST Webbook
cpl	157.30	J/mol×K	275.80	NIST Webbook
dvisc	0.0001611	Pa×s	328.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
dvisc	0.0001480	Pa×s	338.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
dvisc	0.0001411	Pa×s	343.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
dvisc	0.0001543	Pa×s	333.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
dvisc	0.0001332	Pa×s	348.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
dvisc	0.0003893	Pa×s	253.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
dvisc	0.0003661	Pa×s	258.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
dvisc	0.0003439	Pa×s	263.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
dvisc	0.0003201	Pa×s	268.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
dvisc	0.0003023	Pa×s	273.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane

dvisc	0.0002859	Pa×s	278.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
dvisc	0.0002703	Pa×s	283.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
dvisc	0.0002547	Pa×s	288.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
dvisc	0.0002399	Pa×s	293.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
dvisc	0.0002289	Pa×s	298.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
dvisc	0.0002144	Pa×s	303.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
dvisc	0.0002023	Pa×s	308.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
dvisc	0.0001910	Pa×s	313.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
dvisc	0.0001287	Pa×s	353.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
dvisc	0.0001724	Pa×s	323.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
dvisc	0.0001813	Pa×s	318.15	Saturated Liquid Viscosity of Cyclopentane and Isopentane
hfust	5.16	kJ/mol	113.37	NIST Webbook
hfust	5.11	kJ/mol	112.60	NIST Webbook
hfust	5.13	kJ/mol	113.40	NIST Webbook
hfust	5.13	kJ/mol	113.40	NIST Webbook
hfust	5.13	kJ/mol	113.39	NIST Webbook
hvapt	21.50	kJ/mol	350.00	NIST Webbook
hvapt	18.00	kJ/mol	390.00	NIST Webbook
hvapt	12.90	kJ/mol	430.00	NIST Webbook
hvapt	30.20	kJ/mol	245.00	NIST Webbook
hvapt	26.20	kJ/mol	295.00	NIST Webbook
hvapt	24.69	kJ/mol	301.00	NIST Webbook

hvapt	24.83	kJ/mol	293.95	NIST Webbook
hvapt	26.90	kJ/mol	289.00	NIST Webbook
hvapt	28.50	kJ/mol	269.50	NIST Webbook
hvapt	25.20	kJ/mol	380.00	NIST Webbook
hvapt	25.20	kJ/mol	355.50	NIST Webbook
hvapt	24.80	kJ/mol	400.50	NIST Webbook
hvapt	25.30	kJ/mol	436.00	NIST Webbook
hvapt	24.40	kJ/mol	310.00	NIST Webbook
rfi	1.35350		293.15	Isobaric Vapor Liquid Equilibrium for Nine Binary Systems of Cracking C5 Fraction at 250 kPa
sfust	45.24	J/mol×K	113.39	NIST Webbook
sfust	45.23	J/mol×K	113.40	NIST Webbook
sfust	45.41	J/mol×K	112.60	NIST Webbook
sfust	45.48	J/mol×K	113.37	NIST Webbook
svapt	84.48	J/mol×K	293.95	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.45140e+01
Coeff. B	-4.98703e+03
Coeff. C	-7.72933e+00
Coeff. D	8.65422e-06
Temperature range (K), min.	113.25
Temperature range (K), max.	460.43

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid

280.00	200000.00	744.07
280.00	180000.00	737.33
280.00	160000.00	729.89
280.00	140000.00	722.2
280.00	120000.00	713.77
280.00	100000.00	704.35
280.00	90000.00	699.3
280.00	80000.00	694.03
280.00	70000.00	688.43
280.00	60000.00	682.44
280.00	50000.00	675.94
280.00	40000.00	669.03
280.00	30000.00	661.46
280.00	20000.00	653.11
280.00	10000.00	643.42
280.00	5000.00	638.02
280.00	3000.00	635.86
280.00	2000.00	634.7
280.00	1000.00	633.54
300.00	200000.00	734.71
300.00	180000.00	727.5
300.00	160000.00	719.81
300.00	140000.00	711.75
300.00	120000.00	702.76
300.00	100000.00	692.98
300.00	90000.00	687.64
300.00	80000.00	682.03
300.00	70000.00	675.91
300.00	60000.00	669.45
300.00	50000.00	662.36
300.00	40000.00	654.71
300.00	30000.00	646.19
300.00	20000.00	636.61
300.00	10000.00	625.53
300.00	5000.00	619.26
300.00	3000.00	616.54
300.00	2000.00	615.18
300.00	1000.00	613.77
320.00	200000.00	725.65
320.00	180000.00	718.37
320.00	160000.00	710.26
320.00	140000.00	701.5
320.00	120000.00	691.83
320.00	100000.00	681.48

320.00	90000.00	675.83
320.00	80000.00	669.62
320.00	70000.00	662.98
320.00	60000.00	656.03
320.00	50000.00	648.39
320.00	40000.00	639.89
320.00	30000.00	630.46
320.00	20000.00	619.58
320.00	10000.00	606.77
320.00	5000.00	599.33
320.00	3000.00	596.07
320.00	2000.00	594.35
320.00	1000.00	592.72
340.00	200000.00	716.61
340.00	180000.00	708.89
340.00	160000.00	700.49
340.00	140000.00	691.52
340.00	120000.00	681.53
340.00	100000.00	670.52
340.00	90000.00	664.53
340.00	80000.00	658.05
340.00	70000.00	651.03
340.00	60000.00	643.45
340.00	50000.00	635.12
340.00	40000.00	625.82
340.00	30000.00	615.28
340.00	20000.00	602.92
340.00	10000.00	587.99
340.00	5000.00	578.97
340.00	3000.00	574.98
340.00	2000.00	572.85
340.00	1000.00	570.66
360.00	200000.00	708.18
360.00	180000.00	699.47
360.00	160000.00	691.16
360.00	140000.00	681.34
360.00	120000.00	671.11
360.00	100000.00	659.45
360.00	90000.00	652.93
360.00	80000.00	645.89
360.00	70000.00	638.43
360.00	60000.00	630.27
360.00	50000.00	621.15
360.00	40000.00	610.91

360.00	30000.00	599.16
360.00	20000.00	585.18
360.00	10000.00	567.71
360.00	5000.00	556.57
360.00	3000.00	551.5
360.00	2000.00	548.79
360.00	1000.00	545.89
380.00	200000.00	699.6
380.00	180000.00	691.12
380.00	160000.00	682.07
380.00	140000.00	672.14
380.00	120000.00	661.13
380.00	100000.00	648.74
380.00	90000.00	641.88
380.00	80000.00	634.41
380.00	70000.00	626.4
380.00	60000.00	617.61
380.00	50000.00	607.73
380.00	40000.00	596.53
380.00	30000.00	583.41
380.00	20000.00	567.43
380.00	10000.00	546.59
380.00	5000.00	532.71
380.00	3000.00	526.02
380.00	2000.00	522.38
380.00	1000.00	518.39
400.00	200000.00	691.58
400.00	180000.00	682.87
400.00	160000.00	673.54
400.00	140000.00	662.94
400.00	120000.00	651.4
400.00	100000.00	638.47
400.00	90000.00	631.33
400.00	80000.00	623.43
400.00	70000.00	614.87
400.00	60000.00	605.35
400.00	50000.00	594.58
400.00	40000.00	582.37
400.00	30000.00	567.78
400.00	20000.00	549.47
400.00	10000.00	524.35
400.00	5000.00	506.33
400.00	3000.00	497.03
400.00	2000.00	491.59

420.00	200000.00	683.74
420.00	180000.00	674.63
420.00	160000.00	664.82
420.00	140000.00	653.97
420.00	120000.00	641.97
420.00	100000.00	628.24
420.00	90000.00	620.5
420.00	80000.00	612.1
420.00	70000.00	602.84
420.00	60000.00	592.84
420.00	50000.00	581.15
420.00	40000.00	567.85
420.00	30000.00	551.51
420.00	20000.00	530.77
420.00	10000.00	500.48
420.00	5000.00	476.16
420.00	3000.00	461.88
420.00	2000.00	452.61
440.00	200000.00	676.01
440.00	180000.00	666.6
440.00	160000.00	656.44
440.00	140000.00	645.06
440.00	120000.00	632.51
440.00	100000.00	618.08
440.00	90000.00	610.1
440.00	80000.00	601.22
440.00	70000.00	591.44
440.00	60000.00	580.59
440.00	50000.00	568.08
440.00	40000.00	553.42
440.00	30000.00	535.46
440.00	20000.00	511.64
440.00	10000.00	474.4
440.00	5000.00	439.7
440.00	3000.00	412.99
298.14	177400.00	727.57
298.14	101400.00	694.83
298.14	40600.00	656.53
298.14	10200.00	627.35
323.13	196130.00	722.79
323.13	147100.00	703.2
323.13	98070.00	678.79
323.13	49030.00	645.8
368.12	196130.00	703.04

368.12	147100.00	681.34
368.12	98070.00	653.72
320.00	2000.00	595.25
320.00	1000.00	593.5
320.00	502.00	592.61
320.00	315.00	592.25
320.00	210.00	592.07
320.00	199.00	592.04
340.00	1000.00	571.14
340.00	513.00	570.01
340.00	420.00	569.78
340.00	338.00	569.61
360.00	1000.00	545.87
360.00	702.00	545.09
360.00	609.00	544.84
360.00	608.00	544.68
360.00	550.00	544.65
380.00	1001.00	519.03
380.00	962.00	518.87
380.00	857.00	518.44
380.00	846.00	518.39
400.00	2000.00	492.12
400.00	1611.00	489.83
400.00	1506.00	489.2
400.00	1309.00	487.97
400.00	1250.00	487.6
410.00	2000.00	474.02
410.00	1623.00	471.11
410.00	1519.00	470.27
420.00	2000.00	452.93
420.00	1904.00	451.92
420.00	1800.00	450.78
420.00	1789.00	450.66

Reference *https://www.doi.org/10.1016/j.jct.2016.05.019*

Thermal conductivity, W/m/K

Temperature, K - Gas	Pressure, kPa - Gas	Thermal conductivity, W/m/K - Gas
342.97	100.00	0.0195
352.61	100.00	0.0206

375.00	100.00	0.0235
390.75	100.00	0.0257
342.97	200.00	0.0196
352.61	200.00	0.0207
375.00	200.00	0.0236
390.75	200.00	0.0258
342.97	500.00	0.0198
352.61	500.00	0.0209
375.00	500.00	0.0238
390.75	500.00	0.0260

Reference *https://www.doi.org/10.1016/j.fluid.2007.07.059*

Sources

Thermal conductivity of polyurethane foam cell gases: Improved transient hot wire cell data of Isopentane + Cyclopentane mixtures	https://www.doi.org/10.1016/j.fluid.2007.07.059
Isobaric Vapor-Liquid Equilibrium for Nine Binary Systems of Cracking C5 Saturated Linear Hydrocarbons	https://www.doi.org/10.1021/acs.jced.6b00180
Extended Friday-Mason Model for Viscosity of Cyclopentane and Isopentane:	https://www.doi.org/10.1021/je0202174
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Development of a Henry s constant correlation and solubility measurements of n-pentane, i-pentane, cyclopentane, n-hexane, and toluene in water.	https://www.doi.org/10.1016/j.jct.2008.01.019
KDB:	https://www.cheric.org/files/research/kdb/mol/mol33.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=33
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Isobaric vapor-liquid equilibrium for four binary systems of thiophene + 3-methylthiophene:	https://www.doi.org/10.1016/j.fluid.2011.11.020
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78784&Units=SI
Isobaric vapor-liquid equilibrium for four binary systems of 3-methylthiophene:	https://www.doi.org/10.1016/j.fluid.2012.02.005
Liquid-Liquid Equilibria in Ternary Systems 2-Methylbutane + 2-Methyl-2-propanol + Water and 2-Methylpentane + 2-Methyl-2-propanol + Water at 298.15 K:	https://www.doi.org/10.1021/je8004529
The Precise Measurement of Vapor-Liquid Equilibrium Properties of the Pentane + 2-Methyl-2-propanol + Water Ternary Mixture, and Isopentane at T = (280 to 440) K and up to 200 MPa:	https://www.doi.org/10.1007/s10765-017-2283-x
Fitted Parameters for a Helmholtz Energy Mixture Model:	https://www.doi.org/10.1016/j.jct.2016.05.019

Legend

chg:	Standard gas enthalpy of combustion
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
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
ie:	Ionization energy
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
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tcondg:	Gas thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume