

Butane, 1-methoxy-

Other names:	.alpha.-methoxybutane 1-METHOXYBUTANE BUTYL METHYL ETHER Ether, butyl methyl METHYL BUTYL ETHER Methyl n-butyl ether UN 2350 n-Butyl methyl ether n-C4H9OCH3 «alpha»-Methoxybutane Â«alphaÂ»-Methoxybutane
Inchi:	InChI=1S/C5H12O/c1-3-4-5-6-2/h3-5H2,1-2H3
InchiKey:	CXBDYQVECUFKRK-UHFFFAOYSA-N
Formula:	C5H12O
SMILES:	CCCCOC
Mol. weight [g/mol]:	88.15
CAS:	628-28-4

Physical Properties

Property code	Value	Unit	Source
af	0.3160		KDB
affp	820.30	kJ/mol	NIST Webbook
basg	791.20	kJ/mol	NIST Webbook
chl	-3391.99	kJ/mol	NIST Webbook
dm	1.30	debye	KDB
gf	-113.78	kJ/mol	Joback Method
hf	-258.10 ± 1.10	kJ/mol	NIST Webbook
hfl	-290.50 ± 1.30	kJ/mol	NIST Webbook
hfpi	640.00	kJ/mol	NIST Webbook
hfus	9.89	kJ/mol	Joback Method
hvap	32.50 ± 0.10	kJ/mol	NIST Webbook
hvap	32.40	kJ/mol	NIST Webbook
hvap	32.40	kJ/mol	NIST Webbook
hvap	32.53	kJ/mol	NIST Webbook
hvap	32.42	kJ/mol	NIST Webbook
hvap	32.46 ± 0.12	kJ/mol	NIST Webbook
ie	9.54	eV	NIST Webbook

log10ws	-0.99		Estimated Solubility Method
log10ws	-0.99		Aqueous Solubility Prediction Method
logp	1.433		Crippen Method
mcvol	87.180	ml/mol	McGowan Method
pc	3318.00 ± 50.66	kPa	NIST Webbook
pc	3371.00	kPa	KDB
pc	3371.00 ± 8.00	kPa	NIST Webbook
rinpol	601.00		NIST Webbook
rinpol	602.30		NIST Webbook
rinpol	616.00		NIST Webbook
rinpol	616.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	594.00		NIST Webbook
rinpol	604.40		NIST Webbook
ripol	755.00		NIST Webbook
ripol	755.00		NIST Webbook
sg	390.10	J/mol×K	NIST Webbook
sl	295.30	J/mol×K	NIST Webbook
tb	343.00	K	NIST Webbook
tb	335.00 ± 3.00	K	NIST Webbook
tb	343.30	K	NIST Webbook
tb	343.90 ± 1.00	K	NIST Webbook
tb	343.31	K	KDB
tb	344.20	K	NIST Webbook
tc	512.78	K	KDB
tc	512.72 ± 1.00	K	NIST Webbook
tc	512.78 ± 0.10	K	NIST Webbook
tc	512.80	K	NIST Webbook
tf	157.90	K	Aqueous Solubility Prediction Method
tf	157.60	K	KDB
tt	157.48 ± 0.05	K	NIST Webbook
vc	0.329	m3/kmol	KDB
vc	0.329 ± 0.003	m3/kmol	NIST Webbook
zc	0.2601280		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	147.83	J/mol×K	336.22	Joback Method
cpg	156.52	J/mol×K	363.60	Joback Method
cpg	164.99	J/mol×K	390.97	Joback Method
cpg	173.24	J/mol×K	418.35	Joback Method
cpg	181.27	J/mol×K	445.73	Joback Method
cpg	189.09	J/mol×K	473.10	Joback Method
cpg	196.68	J/mol×K	500.48	Joback Method
cpl	192.48	J/mol×K	298.15	NIST Webbook
cpl	192.70	J/mol×K	298.15	NIST Webbook
cpl	193.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0002124	Pa×s	336.22	Joback Method
dvisc	0.0014407	Pa×s	196.32	Joback Method
dvisc	0.0030953	Pa×s	168.34	Joback Method
dvisc	0.0005192	Pa×s	252.28	Joback Method
dvisc	0.0003631	Pa×s	280.26	Joback Method
dvisc	0.0002710	Pa×s	308.24	Joback Method
dvisc	0.0008115	Pa×s	224.30	Joback Method
hfust	10.85	kJ/mol	157.48	NIST Webbook
hfust	10.85	kJ/mol	157.50	NIST Webbook
hfust	10.85	kJ/mol	157.50	NIST Webbook
hvapt	29.55	kJ/mol	343.30	NIST Webbook
hvapt	32.50	kJ/mol	330.00	NIST Webbook
hvapt	29.60	kJ/mol	316.00	NIST Webbook
hvapt	32.40	kJ/mol	319.00	NIST Webbook
pvap	9.21	kPa	283.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures
pvap	5.44	kPa	273.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures

pvap	3.05	kPa	263.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures
pvap	14.93	kPa	293.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures
pvap	18.73	kPa	298.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures
pvap	23.30	kPa	303.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures
pvap	35.15	kPa	313.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures

pvap	51.45	kPa	323.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures
pvap	73.31	kPa	333.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures
pvap	101.96	kPa	343.15	Isothermal vapour liquid equilibria and excess molar enthalpies of hex-2-yne + methyl butyl ether and hex-3-yne + dibutyl ether mixtures
pvap	3.20	kPa	262.99	Isothermal (vapor + liquid) equilibria and excess enthalpy data of {1-hexene + methyl butyl ether (MBE)} and {1-hexene + methyl tert-butyl ether (MTBE)} binary systems at several temperatures
pvap	3.19	kPa	263.15	Isothermal (vapor + liquid) equilibria and excess enthalpy data of {1-hexene + methyl butyl ether (MBE)} and {1-hexene + methyl tert-butyl ether (MTBE)} binary systems at several temperatures

pvap	5.70	kPa	273.04	Isothermal (vapor + liquid) equilibria and excess enthalpy data of {1-hexene + methyl butyl ether (MBE)} and {1-hexene + methyl tert-butyl ether (MTBE)} binary systems at several temperatures
pvap	5.70	kPa	273.15	Isothermal (vapor + liquid) equilibria and excess enthalpy data of {1-hexene + methyl butyl ether (MBE)} and {1-hexene + methyl tert-butyl ether (MTBE)} binary systems at several temperatures
pvap	9.60	kPa	283.07	Isothermal (vapor + liquid) equilibria and excess enthalpy data of {1-hexene + methyl butyl ether (MBE)} and {1-hexene + methyl tert-butyl ether (MTBE)} binary systems at several temperatures
pvap	9.69	kPa	283.15	Isothermal (vapor + liquid) equilibria and excess enthalpy data of {1-hexene + methyl butyl ether (MBE)} and {1-hexene + methyl tert-butyl ether (MTBE)} binary systems at several temperatures
pvap	74.10	kPa	333.25	Isothermal (vapor + liquid) equilibria and excess enthalpy data of {1-hexene + methyl butyl ether (MBE)} and {1-hexene + methyl tert-butyl ether (MTBE)} binary systems at several temperatures

pvap	15.74	kPa	293.15	Isothermal (vapor + liquid) equilibria and excess enthalpy data of {1-hexene + methyl butyl ether (MBE)} and {1-hexene + methyl tert-butyl ether (MTBE)} binary systems at several temperatures
pvap	24.40	kPa	303.12	Isothermal (vapor + liquid) equilibria and excess enthalpy data of {1-hexene + methyl butyl ether (MBE)} and {1-hexene + methyl tert-butyl ether (MTBE)} binary systems at several temperatures
pvap	24.61	kPa	303.15	Isothermal (vapor + liquid) equilibria and excess enthalpy data of {1-hexene + methyl butyl ether (MBE)} and {1-hexene + methyl tert-butyl ether (MTBE)} binary systems at several temperatures
pvap	37.17	kPa	313.15	Isothermal (vapor + liquid) equilibria and excess enthalpy data of {1-hexene + methyl butyl ether (MBE)} and {1-hexene + methyl tert-butyl ether (MTBE)} binary systems at several temperatures

pvap	36.80	kPa	313.16	Isothermal (vapor + liquid) equilibria and excess enthalpy data of {1-hexene + methyl butyl ether (MBE)} and {1-hexene + methyl tert-butyl ether (MTBE)} binary systems at several temperatures
pvap	36.90	kPa	313.16	Isothermal (vapor + liquid) equilibria and excess enthalpy data of {1-hexene + methyl butyl ether (MBE)} and {1-hexene + methyl tert-butyl ether (MTBE)} binary systems at several temperatures
pvap	54.46	kPa	323.15	Isothermal (vapor + liquid) equilibria and excess enthalpy data of {1-hexene + methyl butyl ether (MBE)} and {1-hexene + methyl tert-butyl ether (MTBE)} binary systems at several temperatures
pvap	54.00	kPa	323.20	Isothermal (vapor + liquid) equilibria and excess enthalpy data of {1-hexene + methyl butyl ether (MBE)} and {1-hexene + methyl tert-butyl ether (MTBE)} binary systems at several temperatures
pvap	77.64	kPa	333.15	Isothermal (vapor + liquid) equilibria and excess enthalpy data of {1-hexene + methyl butyl ether (MBE)} and {1-hexene + methyl tert-butyl ether (MTBE)} binary systems at several temperatures

pvap	15.60	kPa	293.10	Isothermal (vapor + liquid) equilibria and excess enthalpy data of {1-hexene + methyl butyl ether (MBE)} and {1-hexene + methyl tert-butyl ether (MTBE)} binary systems at several temperatures
rhoI	744.00	kg/m3	293.00	KDB
sfust	68.90	J/mol×K	157.48	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42391e+01
Coeff. B	-2.87959e+03
Coeff. C	-4.48890e+01
Temperature range (K), min.	251.29
Temperature range (K), max.	367.44

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	8.25169e+01
Coeff. B	-6.53559e+03
Coeff. C	-1.02658e+01
Coeff. D	9.13606e-06
Temperature range (K), min.	285.00
Temperature range (K), max.	508.44

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
283.15	100.00	755.88
288.15	100.00	750.88
293.15	100.00	745.85
298.15	100.00	740.78
303.15	100.00	735.68
308.15	100.00	730.53
313.15	100.00	725.34
318.15	100.00	720.1
323.15	100.00	714.8
328.15	100.00	709.45
333.15	100.00	704.04
283.15	5000.00	760.82
288.15	5000.00	756.01
293.15	5000.00	751.18
298.15	5000.00	746.29
303.15	5000.00	741.39
308.15	5000.00	736.43
313.15	5000.00	731.47
318.15	5000.00	726.46
323.15	5000.00	721.41
328.15	5000.00	716.32
333.15	5000.00	711.19
283.15	10000.00	765.42
288.15	10000.00	760.78
293.15	10000.00	756.08
298.15	10000.00	751.36
303.15	10000.00	746.66
308.15	10000.00	741.88
313.15	10000.00	737.11
318.15	10000.00	732.32
323.15	10000.00	727.49
328.15	10000.00	722.64
333.15	10000.00	717.74
283.15	15000.00	769.77
288.15	15000.00	765.26
293.15	15000.00	760.71
298.15	15000.00	756.15
303.15	15000.00	751.6
308.15	15000.00	746.98

313.15	15000.00	742.4
318.15	15000.00	737.77
323.15	15000.00	733.12
328.15	15000.00	728.5
333.15	15000.00	723.77
283.15	20000.00	773.91
288.15	20000.00	769.53
293.15	20000.00	765.09
298.15	20000.00	760.68
303.15	20000.00	756.25
308.15	20000.00	751.8
313.15	20000.00	747.36
318.15	20000.00	742.89
323.15	20000.00	738.42
328.15	20000.00	733.93
333.15	20000.00	729.38
283.15	25000.00	777.86
288.15	25000.00	773.58
293.15	25000.00	769.27
298.15	25000.00	764.97
303.15	25000.00	760.68
308.15	25000.00	756.35
313.15	25000.00	752.04
318.15	25000.00	747.69
323.15	25000.00	743.37
328.15	25000.00	739.05
333.15	25000.00	734.64
283.15	30000.00	781.65
288.15	30000.00	777.48
293.15	30000.00	773.26
298.15	30000.00	769.08
303.15	30000.00	764.89
308.15	30000.00	760.67
313.15	30000.00	756.48
318.15	30000.00	752.27
323.15	30000.00	748.07
328.15	30000.00	743.83
333.15	30000.00	739.61
283.15	35000.00	785.29
288.15	35000.00	781.19
293.15	35000.00	777.09
298.15	35000.00	772.99
303.15	35000.00	768.9
308.15	35000.00	764.79

313.15	35000.00	760.7
318.15	35000.00	756.62
323.15	35000.00	752.53
328.15	35000.00	748.41
333.15	35000.00	744.31
283.15	40000.00	788.8
288.15	40000.00	784.79
293.15	40000.00	780.75
298.15	40000.00	776.76
303.15	40000.00	772.76
308.15	40000.00	768.74
313.15	40000.00	764.74
318.15	40000.00	760.76
323.15	40000.00	756.76
328.15	40000.00	752.76
333.15	40000.00	748.78
283.15	45000.00	792.18
288.15	45000.00	788.24
293.15	45000.00	784.3
298.15	45000.00	780.38
303.15	45000.00	776.46
308.15	45000.00	772.53
313.15	45000.00	768.63
318.15	45000.00	764.73
323.15	45000.00	760.83
328.15	45000.00	756.92
333.15	45000.00	753.01
283.15	50000.00	795.45
288.15	50000.00	791.57
293.15	50000.00	787.7
298.15	50000.00	783.87
303.15	50000.00	780.03
308.15	50000.00	776.18
313.15	50000.00	772.34
318.15	50000.00	768.51
323.15	50000.00	764.7
328.15	50000.00	760.91
333.15	50000.00	757.06
283.15	55000.00	798.61
288.15	55000.00	794.8
293.15	55000.00	791.0
298.15	55000.00	787.24
303.15	55000.00	783.46
308.15	55000.00	779.69

313.15	55000.00	775.93
318.15	55000.00	772.16
323.15	55000.00	768.43
328.15	55000.00	764.72
333.15	55000.00	760.97
283.15	60000.00	801.68
288.15	60000.00	797.94
293.15	60000.00	794.21
298.15	60000.00	790.51
303.15	60000.00	786.77
308.15	60000.00	783.07
313.15	60000.00	779.39
318.15	60000.00	775.71
323.15	60000.00	772.05
328.15	60000.00	768.39
333.15	60000.00	764.71
283.15	65000.00	804.67
288.15	65000.00	800.98
293.15	65000.00	797.33
298.15	65000.00	793.65
303.15	65000.00	790.0
308.15	65000.00	786.36
313.15	65000.00	782.73
318.15	65000.00	779.13
323.15	65000.00	775.54
328.15	65000.00	771.91
333.15	65000.00	768.34

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Sources

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Aqueous Solubility Prediction Method:

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Phase Separation in Binary Mixtures Containing Linear Perfluoroalkanes:

<https://www.doi.org/10.1021/je049620w>

Experimental and modeled volumetric behavior of linear and branched ethers: KDB Vapor Pressure Data:

<https://www.doi.org/10.1016/j.fluid.2016.02.009>

McGowan Method:

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1005>

<http://link.springer.com/article/10.1007/BF02311772>

Isothermal (vapor + liquid) equilibria and excess enthalpy data of {1-hexene + methyl tert-butyl ether (MTBE)} and {1-hexene + methyl tert-butyl ether (MTBE)} binary systems at several temperatures:

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Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
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
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfpi:	Enthalpy of formation of positive ion 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
rho:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

vc: Critical Volume
zc: Critical Compressibility

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