Butane, 1-(methylthio)-

Other names:	1-(Methylthio)butane
	2-Thiahexane
	Butyl methyl sulfide
	Butyl methyl sulphide
	Butyl methyl thioether
	METHYL N-BUTYL SULFIDE
	Methyl butyl sulfide
	Methyl-n-butyl sulfide
	Sulfide, butyl methyl
	n-Butyl methyl sulfide
	«alpha»-(Methylthio)butane
	Â«alphaÂ»-(Methylthio)butane
Inchi:	InChI=1S/C5H12S/c1-3-4-5-6-2/h3-5H2,1-2H3
InchiKey:	WCXXISMIJBRDQK-UHFFFAOYSA-N
Formula:	C5H12S
SMILES:	CCCCSC
Mol. weight [g/mol]:	104.21
CAS:	628-29-5

Physical Properties

Property code	Value	Unit	Source
chl	-4141.90 ± 0.67	kJ/mol	NIST Webbook
chl	-4141.30 ± 0.67	kJ/mol	NIST Webbook
chl	-4142.10 ± 1.90	kJ/mol	NIST Webbook
gf	24.34	kJ/mol	Joback Method
hf	-102.00	kJ/mol	NIST Webbook
hf	-102.20 ± 1.10	kJ/mol	NIST Webbook
hf	-101.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-142.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-142.80 ± 0.75	kJ/mol	NIST Webbook
hfl	-143.00 ± 0.84	kJ/mol	NIST Webbook
hfus	12.84	kJ/mol	Joback Method
hvap	40.71	kJ/mol	NIST Webbook
hvap	40.70 ± 0.04	kJ/mol	NIST Webbook
hvap	41.00	kJ/mol	NIST Webbook
hvap	41.00 ± 1.00	kJ/mol	NIST Webbook
hvap	40.90 ± 0.80	kJ/mol	NIST Webbook

hvap	41.00	kJ/mol	NIST Webbook
hvap	40.50	kJ/mol	NIST Webbook
hvap	40.80	kJ/mol	NIST Webbook
hvap	40.50	kJ/mol	NIST Webbook
log10ws	-1.80		Crippen Method
logp	2.150		Crippen Method
mcvol	97.660	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
rinpol	820.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	803.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	813.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	813.00		NIST Webbook
ripol	1043.00		NIST Webbook
ripol	1043.00		NIST Webbook
ripol	1032.60		NIST Webbook
ripol	1029.30		NIST Webbook
ripol	1032.60		NIST Webbook
ripol	1051.00		NIST Webbook
sl	307.48	J/mol×K	NIST Webbook
tb	396.45 ± 0.30	K	NIST Webbook
tb	396.40	K	NIST Webbook
tb	396.00	K	NIST Webbook
tb	396.65 ± 0.20	K	NIST Webbook
tb	396.00 ± 3.00	K	NIST Webbook
tb	396.60	K	NIST Webbook
tc	572.69	K	Joback Method
tf	175.25 ± 0.20	K	NIST Webbook
tf	175.32 ± 0.02	K	NIST Webbook
tt	175.29 ± 0.05	K	NIST Webbook
tt	175.30 ± 0.03	K	NIST Webbook
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.36	J/mol×K	541.00	Joback Method
cpg	169.71	J/mol×K	382.58	Joback Method
cpg	179.76	J/mol×K	414.26	Joback Method
cpg	189.45	J/mol×K	445.95	Joback Method
cpg	198.78	J/mol×K	477.63	Joback Method
cpg	207.75	J/mol×K	509.32	Joback Method
cpg	224.63	J/mol×K	572.69	Joback Method
cpl	200.92	J/mol×K	298.15	NIST Webbook
hfust	12.45	kJ/mol	175.60	NIST Webbook
hfust	12.45	kJ/mol	175.30	NIST Webbook
hfust	12.45	kJ/mol	175.60	NIST Webbook
hvapt	38.10	kJ/mol	310.50	NIST Webbook
hvapt	40.40	kJ/mol	360.00	NIST Webbook
hvapt	35.30	kJ/mol	315.50	NIST Webbook
hvapt	38.00	kJ/mol	389.50	NIST Webbook
hvapt	34.47	kJ/mol	396.60	NIST Webbook
sfust	71.03	J/mol×K	175.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43032e+01
Coeff. B	-3.30746e+03
Coeff. C	-5.47920e+01
Temperature range (K), min.	290.78
Temperature range (K), max.	422.63

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.94595e+01
Coeff. B	-7.85527e+03

Coeff. C	-1.10629e+01
Coeff. D	7.34115e-06
Temperature range (K), min.	290.15
Temperature range (K), max.	591.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1830
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1830.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C628295&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
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
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume