Butane, 1,1'-thiobis-

Other names:	(n-C4H9)2S
	1,1'-Thiobisbutane
	5-thianonane
	Butyl monosulfide
	Di-n-butyl sulfide
	Dibutyl sulphide
	NSC 8460
	Sulfide, n-butyl-
	Thianonane-5
	Thiononane-5
	butyl sulfide
	butylthiobutane
	dibutyl sulfide
	dibutyl thioether
	n-Butyl sulfide
	n-Dibutyl sulfide
Inchi:	InChI=1S/C8H18S/c1-3-5-7-9-8-6-4-2/h3-8H2,1-2H3
InchiKey:	HTIRHQRTDBPHNZ-UHFFFAOYSA-N
Formula:	C8H18S
SMILES:	CCCCSCCCC
Mol. weight [g/mol]:	146.30
CAS:	544-40-1

Physical Properties

Property code	Value	Unit	Source
af	0.4044		Cheméo Relay (1.0)
affp	871.80	kJ/mol	NIST Webbook
basg	842.10	kJ/mol	NIST Webbook
chl	-6102.03	kJ/mol	NIST Webbook
chl	-6102.00 ± 1.30	kJ/mol	NIST Webbook
gf	49.60	kJ/mol	Joback Method
hf	-167.40	kJ/mol	NIST Webbook
hf	-167.20	kJ/mol	NIST Webbook
hfl	-220.50 ± 1.50	kJ/mol	NIST Webbook
hfl	-220.70 ± 1.90	kJ/mol	NIST Webbook
hfus	20.61	kJ/mol	Joback Method
hvap	52.96	kJ/mol	NIST Webbook

hvap	40.30	kJ/mol	NIST Webbook
hvap	53.35	kJ/mol	NIST Webbook
hvap	53.35	kJ/mol	NIST Webbook
hvap	54.20 ± 0.80	kJ/mol	NIST Webbook
hvap	53.00	kJ/mol	NIST Webbook
ie	8.22	eV	NIST Webbook
ie	8.40 ± 0.05	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
log10ws	-3.88		Cheméo Relay (1.0)
logp	3.320		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
rinpol	1081.00		NIST Webbook
rinpol	1084.40		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1084.40		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1053.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1055.00		NIST Webbook
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rinpol	1082.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1081.30		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1077.00		NIST Webbook
ripol	1270.60		NIST Webbook
ripol	1270.00		NIST Webbook
ripol	1256.00		NIST Webbook
ripol	1270.00		NIST Webbook
ripol	1254.00		NIST Webbook
ripol	1270.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1289.00		NIST Webbook
ripol	1286.00		NIST Webbook
ripol	1256.60		NIST Webbook
sl	405.09	J/mol×K	NIST Webbook

tb	458.20 ± 0.60	K	NIST Webbook
tb	461.70	K	NIST Webbook
tb	461.95 ± 0.30	K	NIST Webbook
tc	642.51	K	Cheméo Relay (1.0)
tf	221.85	K	KDB
tf	198.12 ± 0.02	K	NIST Webbook
tt	198.13 ± 0.03	K	NIST Webbook
tt	198.13 ± 0.04	K	NIST Webbook
tt	198.13 ± 0.03	K	NIST Webbook
tt	198.13 ± 0.04	K	NIST Webbook
vc	0.525	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.89	J/mol×K	605.88	Joback Method
cpg	362.10	J/mol×K	636.81	Joback Method
cpg	339.17	J/mol×K	574.95	Joback Method
cpg	286.95	J/mol×K	451.22	Joback Method
cpg	300.83	J/mol×K	482.15	Joback Method
cpg	314.15	J/mol×K	513.08	Joback Method
cpg	326.93	J/mol×K	544.01	Joback Method
cpl	284.34	J/mol×K	298.15	NIST Webbook
hfust	19.43	kJ/mol	198.13	NIST Webbook
hfust	19.41	kJ/mol	198.10	NIST Webbook
hfust	19.41	kJ/mol	198.10	NIST Webbook
hfust	19.43	kJ/mol	198.13	NIST Webbook
hvapt	44.80	kJ/mol	338.50	NIST Webbook
hvapt	46.50	kJ/mol	430.00	NIST Webbook
sfust	98.05	J/mol×K	198.13	NIST Webbook
sfust	98.05	J/mol×K	198.13	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43227e+01

Coeff. B	-3.82370e+03
Coeff. C	-6.76820e+01
Temperature range (K), min.	340.12
Temperature range (K), max.	492.01

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.52296e+02
Coeff. B	-1.67842e+04
Coeff. C	-3.51983e+01
Coeff. D	2.22154e-05
Temperature range (K), min.	303.15
Temperature range (K), max.	650.00

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1843

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C544401&Units=SI

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0, beta):

Liquid-Liquid Equilibria of Ternary Systems Sulfide + Octane + Solvents at Different Temperatures: https://www.doi.org/10.1021/je800340v

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1843

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

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

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
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