

Butyl sulfide

Other names:	(n-C4H9)2S 1,1'-THIOBISBUTANE 5-THIANONANE BUTYLTHIOBUTANE Butane, 1,1'-thiobis- Butyl monosulfide Di-n-butyl sulfide Dibutyl sulfide Dibutyl sulphide Dibutyl thioether NSC 8460 Sulfide, n-butyl- Thianonane-5 Thiononane-5 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]:	146.29
CAS:	544-40-1

Physical Properties

Property code	Value	Unit	Source
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	40.30	kJ/mol	NIST Webbook
hvap	54.20 ± 0.80	kJ/mol	NIST Webbook

hvap	53.35	kJ/mol	NIST Webbook
hvap	53.00	kJ/mol	NIST Webbook
hvap	52.96	kJ/mol	NIST Webbook
ie	8.20	eV	NIST Webbook
ie	8.22	eV	NIST Webbook
ie	8.40 ± 0.05	eV	NIST Webbook
log10ws	-3.05		Crippen Method
logp	3.320		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
rinpol	1060.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1084.40		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1084.40		NIST Webbook
rinpol	1088.50		NIST Webbook
rinpol	1078.10		NIST Webbook
rinpol	1081.30		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1059.00		NIST Webbook
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ripol	1289.00		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
sl	405.09	J/mol×K	NIST Webbook
tb	461.95 ± 0.30	K	NIST Webbook
tb	458.20 ± 0.60	K	NIST Webbook

tb	461.70	K	NIST Webbook
tc	636.81	K	Joback Method
tf	221.85	K	KDB
tf	198.12 ± 0.02	K	NIST Webbook
tt	198.13 ± 0.04	K	NIST Webbook
tt	198.13 ± 0.03	K	NIST Webbook
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

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

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
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

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1843
KDB:	https://www.thermo.com/files/research/kdb/mol/mol1843.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemed.com/doc/models/crippen_log10ws
Liquid-Liquid Equilibria of Ternary Systems Sulfide + Octane + Solvents at Different Temperatures:	https://www.doi.org/10.1021/je800340v
Joback Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C544401&Units=SI

Legend

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

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