Butane, 1,1'-thiobis[3-methyl-

Other names:	1-(Isopentylsulfanyl)-3-methylbutane
	2,8-DIMETHYL-5-THIANONANE
	Di(3-methylbutyl) sulfide
	Diisoamyl sulfide
	Diisopentyl sulfide
	Diisopentyl sulphide
	ISOAMYL SULFIDE
	Isopentyl sulfide
Inchi:	InChI=1S/C10H22S/c1-9(2)5-7-11-8-6-10(3)4/h9-10H,5-8H2,1-4H3
InchiKey:	JWEWNTJADCWFRP-UHFFFAOYSA-N
Formula:	C10H22S
SMILES:	CC(C)CCSCCC(C)C
Mol. weight [g/mol]:	174.35
CAS:	544-02-5

Physical Properties

Property code	Value	Unit	Source
chl	-7399.10 ± 2.10	kJ/mol	NIST Webbook
gf	61.56	kJ/mol	Joback Method
hf	-222.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-282.00 ± 2.00	kJ/mol	NIST Webbook
hfus	18.74	kJ/mol	Joback Method
hvap	60.00 ± 2.00	kJ/mol	NIST Webbook
hvap	60.00	kJ/mol	NIST Webbook
log10ws	-3.41		Crippen Method
logp	3.812		Crippen Method
mcvol	168.110	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
rinpol	1197.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1190.00		NIST Webbook
ripol	1359.00		NIST Webbook
tb	489.20	K	NIST Webbook

tb	484.00	K	KDB
tb	488.00 ± 0.70	K	NIST Webbook
tc	664.00	K	KDB
tf	206.86	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.28	J/mol×K	496.10	Joback Method
cpg	392.87	J/mol×K	527.73	Joback Method
cpg	408.74	J/mol×K	559.36	Joback Method
cpg	423.89	J/mol×K	591.00	Joback Method
cpg	438.36	J/mol×K	622.63	Joback Method
cpg	452.14	J/mol×K	654.26	Joback Method
cpg	465.27	J/mol×K	685.89	Joback Method
hvapt	57.90	kJ/mol	352.50	NIST Webbook
hvapt	56.90	kJ/mol	352.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49338e+01
Coeff. B	-4.25050e+03
Coeff. C	-7.71480e+01
Temperature range (K), min.	367.36
Temperature range (K), max.	518.88

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.91108e+00
Coeff. B	-3.24116e+03
Coeff. C	1.27574e-06
Coeff. D	-2.68983e-12

Temperature range (K), min.	283.15
Temperature range (K), max.	353.15

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.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1847
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/mol1847.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C544025&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume