Butane, 2,2'-thiobis-

Other names:	3,5-Dimethyl-4-thiaheptane
	Di-(2-butyl)sulfide
	Di-sec-Butyl thioether
	Di-sec-butyl sulfide
	di-sec-butyl sulphide
	sec-Butyl Sulfide
Inchi:	InChI=1S/C8H18S/c1-5-7(3)9-8(4)6-2/h7-8H,5-6H2,1-4H3
InchiKey:	IEBAOPMEYUWQPD-UHFFFAOYSA-N
Formula:	C8H18S
SMILES:	CCC(C)SC(C)CC
Mol. weight [g/mol]:	146.29
CAS:	626-26-6

Physical Properties

Property code	Value	Unit	Source
gf	44.72	kJ/mol	Joback Method
hf	-177.14	kJ/mol	Joback Method
hfus	13.56	kJ/mol	Joback Method
hvap	43.80 ± 0.10	kJ/mol	NIST Webbook
hvap	47.00	kJ/mol	NIST Webbook
hvap	49.30 ± 0.80	kJ/mol	NIST Webbook
hvap	43.80	kJ/mol	NIST Webbook
log10ws	-3.28		Crippen Method
logp	3.317		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	2621.78	kPa	Joback Method
rinpol	983.00		NIST Webbook
rinpol	983.00		NIST Webbook
tb	438.20	K	NIST Webbook
tc	644.50	K	Joback Method
tf	184.32	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.15	J/mol×K	644.50	Joback Method
cpg	301.81	J/mol×K	482.70	Joback Method
cpg	315.88	J/mol×K	515.06	Joback Method
cpg	329.34	J/mol×K	547.42	Joback Method
cpg	342.19	J/mol×K	579.78	Joback Method
cpg	354.46	J/mol×K	612.14	Joback Method
cpg	287.13	J/mol×K	450.34	Joback Method
hvapt	44.90	kJ/mol	296.50	NIST Webbook
hvapt	41.40	kJ/mol	399.50	NIST Webbook
hvapt	46.40	kJ/mol	430.00	NIST Webbook
hvapt	44.80	kJ/mol	293.00	NIST Webbook
hvapt	42.40	kJ/mol	372.00	NIST Webbook
hvapt	42.30	kJ/mol	337.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48389e+01
Coeff. B	-3.83519e+03
Coeff. C	-6.29560e+01
Temperature range (K), min.	326.52
Temperature range (K), max.	465.50

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C626266&Units=SI

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

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

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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume