Propane, 1,1'-thiobis[2-methyl-

Other names:	(iso-C4H9)2S
	1,1'-Thiobis(2-methyl-propane)
	2,6-Dimethyl-4-thiaheptane
	DI-ISO-BUTYL SULFIDE
	Di(2-methylpropyl) sulfide
	Diisobutyl sulfide
	Diisobutyl sulphide
	Isobutyl sulfide
	Sulfide, diisobutyl-
Inchi:	InChI=1S/C8H18S/c1-7(2)5-9-6-8(3)4/h7-8H,5-6H2,1-4H3
InchiKey:	CMWSRWTXVQLHNX-UHFFFAOYSA-N
Formula:	C8H18S
SMILES:	CC(C)CSCC(C)C
Mol. weight [g/mol]:	146.29
CAS:	592-65-4

Physical Properties

Property code	Value	Unit	Source
chl	-6093.20 ± 1.50	kJ/mol	NIST Webbook
gf	44.72	kJ/mol	Joback Method
hf	-179.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-229.00 ± 2.00	kJ/mol	NIST Webbook
hfus	13.56	kJ/mol	Joback Method
hvap	50.00 ± 2.00	kJ/mol	NIST Webbook
hvap	48.70	kJ/mol	NIST Webbook
hvap	50.00	kJ/mol	NIST Webbook
hvap	48.71	kJ/mol	NIST Webbook
hvap	48.50 ± 0.80	kJ/mol	NIST Webbook
ie	8.36 ± 0.05	eV	NIST Webbook
ie	8.32	eV	NIST Webbook
log10ws	-2.57		Crippen Method
logp	3.032		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	2621.78	kPa	Joback Method
rinpol	997.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	1003.00		NIST Webbook

rinpol	983.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	994.00		NIST Webbook
ripol	1149.00		NIST Webbook
ripol	1149.00		NIST Webbook
tb	447.00 ± 2.00	K	NIST Webbook
tb	445.20 ± 0.60	K	NIST Webbook
tb	445.50 ± 0.50	K	NIST Webbook
tc	644.50	K	Joback Method
tf	167.65 ± 0.50	K	NIST Webbook
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.13	J/mol×K	450.34	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	366.15	J/mol×K	644.50	Joback Method
hvapt	46.40	kJ/mol	335.50	NIST Webbook
hvapt	43.10	kJ/mol	336.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47339e+01
Coeff. B	-3.85276e+03
Coeff. C	-6.46240e+01
Temperature range (K), min.	331.32
Temperature range (K), max.	473.52

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.72060e+01
Coeff. B	-5.56944e+03
Coeff. C	3.06876e-02
Coeff. D	-4.48340e-08
Temperature range (K), min.	325.15
Temperature range (K), max.	346.15

Sources

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/mol1844.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C592654&Units=SI
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=1844
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume