Propane, 2-(methylthio)-

Other names:	2-(METHYLTHIO)PROPANE
	3-METHYL-2-THIABUTANE
	Isopropyl methyl sulfide
	Isopropyl methyl sulphide
	Methyl isopropyl sulfide
	Sulfide, isopropyl methyl
Inchi:	InChI=1S/C4H10S/c1-4(2)5-3/h4H,1-3H3
InchiKey:	ROSSIHMZZJOVOU-UHFFFAOYSA-N
Formula:	C4H10S
SMILES:	CSC(C)C
Mol. weight [g/mol]:	90.19
CAS:	1551-21-9

Physical Properties

Property code	Value	Unit	Source
af	0.2590		KDB
chl	-3480.80 ± 0.59	kJ/mol	NIST Webbook
gf	13.48	kJ/mol	Joback Method
hf	-89.66 ± 0.75	kJ/mol	NIST Webbook
hfl	-124.70 ± 0.75	kJ/mol	NIST Webbook
hfus	6.72	kJ/mol	Joback Method
hvap	35.00	kJ/mol	NIST Webbook
hvap	34.10	kJ/mol	NIST Webbook
hvap	34.24	kJ/mol	NIST Webbook
hvap	34.20	kJ/mol	NIST Webbook
ie	8.70 ± 0.20	eV	NIST Webbook
log10ws	-1.49		Crippen Method
logp	1.758		Crippen Method
mcvol	83.570	ml/mol	McGowan Method
pc	3900.00	kPa	KDB
rinpol	650.00		NIST Webbook
rinpol	675.00		NIST Webbook
rinpol	675.00		NIST Webbook
rinpol	675.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	675.00		NIST Webbook

sl	263.09	J/mol×K	NIST Webbook
tb	357.90	K	KDB
tc	549.50	K	NIST Webbook
tc	551.00	K	KDB
tf	172.00	K	KDB
tf	171.64 ± 0.06	K	NIST Webbook
tf	171.67 ± 0.10	K	NIST Webbook
tt	171.65 ± 0.06	K	NIST Webbook
vc	0.307	m3/kmol	KDB
zc	0.2617710		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.53	J/mol×K	555.15	Joback Method
cpg	144.14	J/mol×K	391.91	Joback Method
cpg	152.64	J/mol×K	424.56	Joback Method
cpg	160.82	J/mol×K	457.20	Joback Method
cpg	168.70	J/mol×K	489.85	Joback Method
cpg	176.26	J/mol×K	522.50	Joback Method
cpg	135.33	J/mol×K	359.26	Joback Method
cpl	172.38	J/mol×K	298.15	NIST Webbook
hfust	9.36	kJ/mol	171.70	NIST Webbook
hfust	9.36	kJ/mol	171.65	NIST Webbook
hfust	9.36	kJ/mol	171.70	NIST Webbook
hvapt	30.70	kJ/mol	357.90	KDB
hvapt	30.71	kJ/mol	357.90	NIST Webbook
hvapt	33.80	kJ/mol	333.00	NIST Webbook
hvapt	33.00 ± 0.10	kJ/mol	318.00	NIST Webbook
hvapt	32.00 ± 0.10	kJ/mol	336.00	NIST Webbook
hvapt	30.70 ± 0.10	kJ/mol	358.00	NIST Webbook
sfust	54.50	J/mol×K	171.65	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.40173e+01
Coeff. B	-2.92160e+03
Coeff. C	-4.81570e+01
Temperature range (K), min.	260.95
Temperature range (K), max.	383.75

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.92492e+01
Coeff. B	-6.63680e+03
Coeff. C	-9.70503e+00
Coeff. D	7.65631e-06
Temperature range (K), min.	260.15
Temperature range (K), max.	551.00

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1551219&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=1824

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/mol1824.mol

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

Legend

af: Acentric Factor

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
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
zc:	Critical Compressibility