Benzene, (methylthio)-

Other names:	(1-Thiaethyl)benzene
	(Methylthio)benzene
	1-Phenyl-1-thiaethane
	Anisole, thio-
	Methyl phenyl sulfide
	Methyl phenyl sulphide
	NSC 57916
	Phenyl methyl sulfide
	Phenylthiomethane
	Sulfide, methyl phenyl
	Thioanisol
	Thioanisole
Inchi:	InChI=1S/C7H8S/c1-8-7-5-3-2-4-6-7/h2-6H,1H3
InchiKey:	HNKJADCVZUBCPG-UHFFFAOYSA-N
Formula:	C7H8S
SMILES:	CSc1ccccc1
Mol. weight [g/mol]:	124.20
CAS:	100-68-5

Physical Properties

Property code	Value	Unit	Source
affp	872.60	kJ/mol	NIST Webbook
basg	843.70	kJ/mol	NIST Webbook
chl	-4543.20 ± 3.60	kJ/mol	NIST Webbook
chl	-4547.80 ± 2.00	kJ/mol	NIST Webbook
gf	153.59	kJ/mol	Joback Method
hf	98.00 ± 3.00	kJ/mol	NIST Webbook
hf	97.28 ± 0.84	kJ/mol	NIST Webbook
hfl	43.30 ± 0.71	kJ/mol	NIST Webbook
hfl	48.00 ± 2.00	kJ/mol	NIST Webbook
hfus	12.06	kJ/mol	Joback Method
hvap	40.27	kJ/mol	Joback Method
ie	8.04	eV	NIST Webbook
ie	7.90 ± 0.15	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	8.07	eV	NIST Webbook
ie	7.92 ± 0.02	eV	NIST Webbook

ie	8.08	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.07	eV	NIST Webbook
ie	8.07	eV	NIST Webbook
ie	7.96 ± 0.01	eV	NIST Webbook
ie	7.93	eV	NIST Webbook
ie	7.94 ± 0.02	eV	NIST Webbook
ie	8.02	eV	NIST Webbook
log10ws	-2.39		Aqueous Solubility Prediction Method
log10ws	-2.39		Estimated Solubility Method
logp	2.409		Crippen Method
mcvol	102.080	ml/mol	McGowan Method
pc	4050.00	kPa	Critical Point and Vapor Pressure Measurements for Seven Compounds by a Low Residence Time Flow Method
rinpol	1106.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1106.00		NIST Webbook
ripol	1574.00		NIST Webbook
sl	252.50	J/mol×K	NIST Webbook
tb	467.00 ± 3.00	K	NIST Webbook
tb	459.00 ± 4.00	K	NIST Webbook
tb	461.20	K	NIST Webbook
tc	693.79	K	Joback Method
tf	229.47	K	Joback Method
tt	256.44 ± 0.01	K	NIST Webbook
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.48	J/mol×K	693.79	Joback Method
cpg	194.62	J/mol×K	494.82	Joback Method
cpg	205.83	J/mol×K	534.61	Joback Method
cpg	216.30	J/mol×K	574.41	Joback Method
cpg	226.04	J/mol×K	614.20	Joback Method
cpg	235.09	J/mol×K	654.00	Joback Method
cpg	182.64	J/mol×K	455.02	Joback Method

cpl	206.02	J/mol×K	298.15	NIST Webbook
hfust	14.84	kJ/mol	256.44	NIST Webbook
hfust	14.85	kJ/mol	256.40	NIST Webbook
hfust	14.85	kJ/mol	256.40	NIST Webbook
hvapt	47.50	kJ/mol	432.00	NIST Webbook
sfust	57.85	J/mol×K	256.44	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47793e+01
Coeff. B	-3.96663e+03
Coeff. C	-7.08200e+01
Temperature range (K), min.	344.54
Temperature range (K), max.	489.78

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C100685&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

Critical Point and Vapor Pressure Measurements for Seven Compounds by a Low Residence Time Flow Method: https://www.doi.org/10.1021/je060088h

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

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