Benzenethiol

Other names:	930-69-8
	Mercaptobenzene
	NSC 6953
	PHENYL MERCAPTANE
	Phenol, thio-
	Phenyl mercaptan
	Phenylthiol
	Rcra waste number P014
	THIOPHENOL
	Thiofenol
	UN 2337
	USAF XR-19
Inchi:	InChI=1S/C6H6S/c7-6-4-2-1-3-5-6/h1-5,7H
InchiKey:	RMVRSNDYEFQCLF-UHFFFAOYSA-N
Formula:	C6H6S
SMILES:	Sc1ccccc1
Mol. weight [g/mol]:	110.18
CAS:	108-98-5

Physical Properties

Property code	Value	Unit	Source
af	0.2940		KDB
chl	-3884.60 ± 0.63	kJ/mol	NIST Webbook
gf	141.44	kJ/mol	Joback Method
hf	112.40 ± 0.88	kJ/mol	NIST Webbook
hfl	63.68 ± 0.84	kJ/mol	NIST Webbook
hfus	9.38	kJ/mol	Joback Method
hvap	48.70	kJ/mol	NIST Webbook
hvap	47.56	kJ/mol	NIST Webbook
ie	9.00 ± 0.10	eV	NIST Webbook
ie	8.28	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
ie	8.30 ± 0.05	eV	NIST Webbook
ie	8.30 ± 0.01	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.49	eV	NIST Webbook

ie	8.47	eV	NIST Webbook
ie	8.36	eV	NIST Webbook
ie	8.32 ± 0.01	eV	NIST Webbook
log10ws	-2.12		Aqueous Solubility Prediction Method
log10ws	-2.12		Estimated Solubility Method
logp	1.975		Crippen Method
mcvol	87.990	ml/mol	McGowan Method
pc	4600.00	kPa	KDB
rinpol	999.00		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	966.00		NIST Webbook
ripol	1491.00		NIST Webbook
sl	222.80	J/mol×K	NIST Webbook
sl	220.10	J/mol×K	NIST Webbook
tb	442.30	K	KDB
tb	442.25 ± 0.20	K	NIST Webbook
tb	442.60	K	NIST Webbook
tb	441.90	K	NIST Webbook
tb	442.70 ± 0.50	K	NIST Webbook
tb	442.30	K	NIST Webbook
tc	689.50	K	NIST Webbook
tc	685.00	K	KDB
tf	258.00	K	KDB
tf	249.85	K	Aqueous Solubility Prediction Method
tf	258.21 ± 0.02	K	NIST Webbook
tf	258.25 ± 0.15	K	NIST Webbook
tf	258.30 ± 0.20	K	NIST Webbook
tt	258.20 ± 0.20	K	NIST Webbook
tt	258.27	K	KDB
tt	258.27 ± 0.05	K	NIST Webbook
vc	0.318	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	143.35	J/mol×K	426.22	Joback Method
cpg	188.62	J/mol×K	628.67	Joback Method

cpg	180.92	J/mol×K	588.18	Joback Method
cpg	172.58	J/mol×K	547.69	Joback Method
cpg	163.56	J/mol×K	507.20	Joback Method
cpg	153.83	J/mol×K	466.71	Joback Method
cpg	195.71	J/mol×K	669.16	Joback Method
cpl	176.56	J/mol×K	298.10	NIST Webbook
cpl	173.22	J/mol×K	298.15	NIST Webbook
hfust	11.48	kJ/mol	258.20	NIST Webbook
hfust	11.48	kJ/mol	258.20	NIST Webbook
hfust	11.45	kJ/mol	258.27	NIST Webbook
hfust	11.48	kJ/mol	258.20	NIST Webbook
hvapt	43.80 ± 0.10	kJ/mol	375.00	NIST Webbook
hvapt	48.70 ± 0.20	kJ/mol	375.00	NIST Webbook
hvapt	44.30	kJ/mol	382.00	NIST Webbook
hvapt	41.30 ± 0.10	kJ/mol	417.00	NIST Webbook
hvapt	41.80 ± 0.10	kJ/mol	407.00	NIST Webbook
hvapt	42.60 ± 0.10	kJ/mol	395.00	NIST Webbook
hvapt	43.10	kJ/mol	435.50	NIST Webbook
hvapt	45.90	kJ/mol	402.00	NIST Webbook
hvapt	39.93	kJ/mol	442.30	NIST Webbook
hvapt	40.59	kJ/mol	442.30	KDB
sfust	44.45	J/mol×K	258.20	NIST Webbook
sfust	44.32	J/mol×K	258.27	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.00	K	4.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42760e+01
Coeff. B	-3.57716e+03
Coeff. C	-7.15030e+01
Temperature range (K), min.	327.23

Temperature range (K), max.	470.54

Sources

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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1853
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108985&Units=SI

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
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
tbrp:	Boiling point at reduced pressure

tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume