Benzenecarbothioic acid

Other names:	Benzoic acid, thio-
	Benzoyl thiol
	Monothiobenzoic acid
	Thiobenzoic acid
	Acido mercaptobenzoico
Inchi:	InChI=1S/C7H6OS/c8-7(9)6-4-2-1-3-5-6/h1-5H,(H,8,9)
InchiKey:	UIJGNTRUPZPVNG-UHFFFAOYSA-N
Formula:	C7H6OS
SMILES:	O=C(S)c1ccccc1
Mol. weight [g/mol]:	138.19
CAS:	98-91-9

Physical Properties

Property code	Value	Unit	Source
gf	20.94	kJ/mol	Joback Method
hf	-25.38	kJ/mol	Joback Method
hfus	13.57	kJ/mol	Joback Method
hvap	46.94	kJ/mol	Joback Method
ie	9.60	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
log10ws	-2.28		Crippen Method
logp	1.757		Crippen Method
mcvol	103.650	ml/mol	McGowan Method
pc	4876.56	kPa	Joback Method
tb	502.97	K	Joback Method
tc	753.25	K	Joback Method
tf	281.46	K	Joback Method
vc	0.380	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.06	J/mol×K	502.97	Joback Method
cpg	204.74	J/mol×K	544.68	Joback Method

cpg	214.60	J/mol×K	586.40	Joback Method
cpg	223.67	J/mol×K	628.11	Joback Method
cpg	232.00	J/mol×K	669.82	Joback Method
cpg	239.61	J/mol×K	711.54	Joback Method
cpg	246.57	J/mol×K	753.25	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C98919&Units=SI

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

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

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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume