Benzenethiol, 4-bromo-

Other names:	Benzenethiol, p-bromo-
	p-Bromobenzenethiol
	p-Bromophenyl thiol
	p-Bromothiophenol
	4-Bromobenzenethiol
Inchi:	InChI=1S/C6H5BrS/c7-5-1-3-6(8)4-2-5/h1-4,8H
InchiKey:	FTBCOQFMQSTCQQ-UHFFFAOYSA-N
Formula:	C6H5BrS
SMILES:	Sc1ccc(Br)cc1
Mol. weight [g/mol]:	189.07
CAS:	106-53-6

Physical Properties

Property code	Value	Unit	Source
gf	146.13	kJ/mol	Joback Method
hf	122.70	kJ/mol	Joback Method
hfus	14.28	kJ/mol	Joback Method
hvap	45.06	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.738		Crippen Method
mcvol	105.490	ml/mol	McGowan Method
pc	5527.84	kPa	Joback Method
tb	512.00	K	NIST Webbook
tb	512.20	K	NIST Webbook
tc	761.63	K	Joback Method
tf	348.00	K	NIST Webbook
vc	0.380	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.21	J/mol×K	497.36	Joback Method
cpg	182.36	J/mol×K	541.40	Joback Method
cpg	190.75	J/mol×K	585.45	Joback Method

cpg	198.42	J/mol×K	629.49	Joback Method
cpg	205.42	J/mol×K	673.54	Joback Method
cpg	211.82	J/mol×K	717.58	Joback Method
cpg	217.66	J/mol×K	761.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106536&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
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