Benzene, 1-bromo-4-(methylthio)-

Other names:	p-Bromo(methylthio)benzene
	1-Bromo-4-(methylthio)benzene
	4-Bromo(methylthio)benzene
	p-Bromophenyl methyl sulfide
	4-Bromophenyl methyl sulfide
	p-Bromothioanisole
	4-Bromothioanisole
	p-(Methylthio)phenyl bromide
	Sulfide, p-bromophenyl methyl
	Methyl 4-bromophenylsulfide
	NSC 73383
	4-bromophenyl methyl sulphide
Inchi:	InChI=1S/C7H7BrS/c1-9-7-4-2-6(8)3-5-7/h2-5H,1H3
InchiKey:	YEUYZNNBXLMFCW-UHFFFAOYSA-N
Formula:	C7H7BrS
SMILES:	CSc1ccc(Br)cc1
Mol. weight [g/mol]:	203.10
CAS:	104-95-0

Physical Properties

Property code	Value	Unit	Source
gf	158.28	kJ/mol	Joback Method
hf	105.45	kJ/mol	Joback Method
hfus	16.95	kJ/mol	Joback Method
hvap	47.37	kJ/mol	Joback Method
ie	7.80	eV	NIST Webbook
ie	8.17 ± 0.05	eV	NIST Webbook
ie	7.50	eV	NIST Webbook
log10ws	-3.38		Crippen Method
logp	3.171		Crippen Method
mcvol	119.580	ml/mol	McGowan Method
pc	4516.42	kPa	Joback Method
tb	528.00	K	NIST Webbook
tc	784.10	K	Joback Method
tf	312.00 ± 1.00	K	NIST Webbook
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.93	J/mol×K	526.16	Joback Method
cpg	225.61	J/mol×K	569.15	Joback Method
cpg	235.48	J/mol×K	612.14	Joback Method
cpg	244.59	J/mol×K	655.13	Joback Method
cpg	252.98	J/mol×K	698.12	Joback Method
cpg	260.67	J/mol×K	741.11	Joback Method
cpg	267.71	J/mol×K	784.10	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104950&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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