

Benzene, 1-bromo-2-(methylthio)-

Other names:	o-Bromo(methylthio)benzene o-Bromophenyl methyl sulfide o-Bromothioanisole Sulfide, o-bromophenyl methyl 2-Bromothioanisole
Inchi:	InChI=1S/C7H7BrS/c1-9-7-5-3-2-4-6(7)8/h2-5H,1H3
InchiKey:	ALAQDUSTXPEHMH-UHFFFAOYSA-N
Formula:	C7H7BrS
SMILES:	CSc1ccccc1Br
Mol. weight [g/mol]:	203.10
CAS:	19614-16-5

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
log10ws	-3.38		Crippen Method
logp	3.171		Crippen Method
mcvol	119.580	ml/mol	McGowan Method
pc	4516.42	kPa	Joback Method
tb	526.16	K	Joback Method
tc	784.10	K	Joback Method
tf	248.60	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	418.70	K	3.60	NIST Webbook
tbrp	529.00	K	102.00	NIST Webbook
tbrp	448.50 ± 3.50	K	1.80	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19614165&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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