2-Bromothioanisole

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

Physical Properties

Property code	Value	Unit	Source
hfus	16.95	kJ/mol	Joback Method
ie	8.28	eV	Cheméo Relay (1.0)
log10ws	-3.39		Cheméo Relay (1.0)
logp	3.171		Crippen Method
mcvol	119.580	ml/mol	McGowan Method
tb	523.29	K	Cheméo Relay (1.0)
tf	248.60	K	NIST Webbook

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19614165&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point