3-Bromophenyl isothiocyanate

Other names:	Isothiocyanic acid, m-bromophenyl ester
	Benzene, 1-bromo-3-isothiocyanato-
	m-Bromophenyl isothiocyanate
Inchi:	InChI=1S/C7H4BrNS/c8-6-2-1-3-7(4-6)9-5-10/h1-4H
InchiKey:	ZMGMGHNOACSMQN-UHFFFAOYSA-N
Formula:	C7H4BrNS
SMILES:	S=C=Nc1cccc(Br)c1
Mol. weight [g/mol]:	214.08
CAS:	2131-59-1

Physical Properties

Property code	Value	Unit	Source
hf	347.65	kJ/mol	Joback Method
hvap	50.99	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.183		Crippen Method
mcvol	120.960	ml/mol	McGowan Method
pc	4546.92	kPa	Joback Method
tb	603.33	K	Joback Method
tc	885.26	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2131591&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

hf:	Enthalpy of formation 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