Benzene, 1-bromo-4-isothiocyanato-2-methyl-

Other names: 2-bromo-5-isothiocyanatotoluene
Inchi: InChI=1S/C8H6BrNS/c1-6-4-7(10-5-11)2-3-8(6)9/h2-4H,1H3
InchiKey: RXWYFLRAEYPAIV-UHFFFAOYSA-N
Formula: C8H6BrNS
SMILES: Cc1cc(N=C=S)ccc1Br
Mol. weight [g/mol]: 228.11
CAS: 71672-88-3

Physical Properties

Property code	Value	Unit	Source
hf	315.54	kJ/mol	Joback Method
hvap	53.88	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.492		Crippen Method
mcvol	135.050	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
tb	631.19	K	Joback Method
tc	906.91	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C71672883&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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