

# 4-Bromo-2,6-dimethylphenyl isothiocyanate

**Inchi:** InChI=1S/C9H8BrNS/c1-6-3-8(10)4-7(2)9(6)11-5-12/h3-4H,1-2H3  
**InchiKey:** CAANWLMQHPUROR-UHFFFAOYSA-N  
**Formula:** C9H8BrNS  
**SMILES:** Cc1cc(Br)cc(C)c1N=C=S  
**Mol. weight [g/mol]:** 242.14  
**CAS:** 77159-76-3

## Physical Properties

Property code	Value	Unit	Source
hf	283.43	kJ/mol	Joback Method
hvap	56.77	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.800		Crippen Method
mcvol	149.140	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
tb	659.05	K	Joback Method
tc	928.74	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C77159763&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/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

<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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