

# 2,3-Dibromopropyl isothiocyanate

**Inchi:** InChI=1S/C4H5Br2NS/c5-1-4(6)2-7-3-8/h4H,1-2H2  
**InchiKey:** AFQQAQKQKFCSPQ-UHFFFAOYSA-N  
**Formula:** C4H5Br2NS  
**SMILES:** S=C=NCC(Br)CBr  
**Mol. weight [g/mol]:** 258.96  
**CAS:** 51784-10-2

## Physical Properties

Property code	Value	Unit	Source
hf	205.56	kJ/mol	Joback Method
hvap	47.42	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.248		Crippen Method
mcvol	119.950	ml/mol	McGowan Method
pc	4862.97	kPa	Joback Method
tb	568.75	K	Joback Method
tc	829.11	K	Joback Method

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C51784102&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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

Latest version available from:

<https://www.cheméo.com/cid/21-479-7/2-3-Dibromopropyl-isothiocyanate.pdf>

Generated by Cheméo on 2024-05-01 22:12:26.753850517 +0000 UTC m=+16890795.674427832.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.