# 2-Propenethioamide, 3-(4-bromophenyl)-2-cyano-, (E)-

**Inchi:** InChI=1S/C10H7BrN2S/c11-9-3-1-7(2-4-9)5-8(6-12)10(13)14/h1-5H,(H2,13,14)/b8-5+

**InchiKey:** JOJTVFIVYQYWGX-VMPITWQZSA-N

**Formula:** C10H7BrN2S

**SMILES:** N#CC(=Cc1ccc(Br)cc1)C(N)=S

**Mol. weight [g/mol]:** 267.14

**CAS:** 68029-54-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 538.78 | kJ/mol | Joback Method |
| hf | 454.26 | kJ/mol | Joback Method |
| hfus | 30.79 | kJ/mol | Joback Method |
| hvap | 75.11 | kJ/mol | Joback Method |
| log10ws | -4.45 | | Crippen Method |
| logp | 2.642 | | Crippen Method |
| mcvol | 164.610 | ml/mol | McGowan Method |
| pc | 3848.31 | kPa | Joback Method |
| tb | 774.71 | K | Joback Method |
| tc | 1053.77 | K | Joback Method |
| tf | 464.68 | K | Joback Method |
| vc | 0.622 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 363.05 | J/mol×K | 774.71 | Joback Method |
| cpg | 371.18 | J/mol×K | 821.22 | Joback Method |
| cpg | 378.79 | J/mol×K | 867.73 | Joback Method |
| cpg | 386.08 | J/mol×K | 914.24 | Joback Method |
| cpg | 393.21 | J/mol×K | 960.75 | Joback Method |
| cpg | 400.37 | J/mol×K | 1007.26 | Joback Method |
| cpg | 407.74 | J/mol×K | 1053.77 | Joback Method |

# Sources

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|---|---|
| **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=C68029549&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion 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 |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |