# 3-Bromomethyl-6-bromo-7-sulfamoyl-3,4-dihydro-

**Inchi:** InChI=1S/C8H9Br2N3O4S2/c9-3-8-12-5-1-4(10)6(18(11,14)15)2-7(5)19(16,17)13-8/h1-2
**InchiKey:** UHLKDFTWNQPIKF-UHFFFAOYSA-N
**Formula:** C8H9Br2N3O4S2
**SMILES:** NS(=O)(=O)c1cc2c(cc1Br)NC(CBr)NS2(=O)=O
**Mol. weight [g/mol]:** 435.11
**CAS:** 3764-20-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -511.18 | kJ/mol | Joback Method |
| hf | -680.93 | kJ/mol | Joback Method |
| hfus | 62.62 | kJ/mol | Joback Method |
| hvap | 111.04 | kJ/mol | Joback Method |
| log10ws | -3.15 | | Crippen Method |
| logp | 0.521 | | Crippen Method |
| mcvol | 210.080 | ml/mol | McGowan Method |
| pc | 9744.98 | kPa | Joback Method |
| tb | 811.63 | K | Joback Method |
| tc | 1062.41 | K | Joback Method |
| tf | 797.41 | K | Joback Method |
| vc | 0.795 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 507.63 | J/mol×K | 811.63 | Joback Method |
| cpg | 517.01 | J/mol×K | 853.43 | Joback Method |
| cpg | 525.21 | J/mol×K | 895.22 | Joback Method |
| cpg | 532.25 | J/mol×K | 937.02 | Joback Method |
| cpg | 538.14 | J/mol×K | 978.82 | Joback Method |
| cpg | 542.88 | J/mol×K | 1020.61 | Joback Method |
| cpg | 546.49 | J/mol×K | 1062.41 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C3764203&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

| | |
|---|---|
| **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 |