# 3H-1,2-Dithiole-3-thione, 5-phenyl-

**Inchi:** InChI=1S/C9H6S3/c10-9-6-8(11-12-9)7-4-2-1-3-5-7/h1-6H
**InchiKey:** NYJHOCZVKHRRLG-UHFFFAOYSA-N
**Formula:** C9H6S3
**SMILES:** S=c1cc(-c2ccccc2)ss1
**Mol. weight [g/mol]:** 210.34
**CAS:** 3445-76-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -6392.00 ± 10.00 | kJ/mol | NIST Webbook |
| hf | 310.00 | kJ/mol | NIST Webbook |
| hfs | 187.00 ± 10.00 | kJ/mol | NIST Webbook |
| hsub | 123.30 | kJ/mol | NIST Webbook |
| hsub | 123.00 | kJ/mol | NIST Webbook |
| hsub | 123.30 ± 0.40 | kJ/mol | NIST Webbook |
| ie | 7.80 | eV | NIST Webbook |
| ie | 8.11 | eV | NIST Webbook |
| log10ws | -4.44 | | Crippen Method |
| logp | 4.206 | | Crippen Method |
| mcvol | 143.500 | ml/mol | McGowan Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| hfust | 26.27 | kJ/mol | 398.00 | NIST Webbook |
| hsubt | 117.40 ± 0.40 | kJ/mol | 368.00 | NIST Webbook |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C3445769&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

| | |
|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase enthalpy of formation at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hsub:** | Enthalpy of sublimation at standard conditions |
| **hsubt:** | Enthalpy of sublimation at a given temperature |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |