# [1,2]Dithiolo[1,5-b][1,2]dithiole-7-S(IV)

| | |
|---|---|
| **Other names:** | Meribicyclo-1,3-epidithiopenta-1,3-diene-5-thial |
| | Thiathiophthen |
| | Thiathiophthene |
| | Thiothiophthene |
| | Trithiapentalene |
| | 1,6,6a-Trithia(6a-SIV)pentalene |
| | 1,6,6a-Trithiapentalene-6«alpha»-S(IV) |
| | 1,6,6a-Trithiapentalene-6aS |
| | 1,6,6aS(IV)-Trithiapentalene |
| | 6a-Thiathiophthene |
| | [1,2]Dithiolo[1,5-b][1,2]dithiole |
| **Inchi:** | InChI=1S/C5H4S3/c1-3-6-8-5(1)2-4-7-8/h1-4H |
| **InchiKey:** | JUEJPBZMWHMMPS-UHFFFAOYSA-N |
| **Formula:** | C5H4S3 |
| **SMILES:** | C1=CC2=S(S1)SC=C2 |
| **Mol. weight [g/mol]:** | 160.28 |
| **CAS:** | 252-09-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 236.41 | kJ/mol | Joback Method |
| hf | 240.38 | kJ/mol | Joback Method |
| hfus | 10.59 | kJ/mol | Joback Method |
| hvap | 46.49 | kJ/mol | Joback Method |
| ie | 8.11 | eV | NIST Webbook |
| log10ws | -3.62 | | Crippen Method |
| logp | 2.779 | | Crippen Method |
| mcvol | 100.040 | ml/mol | McGowan Method |
| pc | 5836.07 | kPa | Joback Method |
| tb | 492.23 | K | Joback Method |
| tc | 778.64 | K | Joback Method |
| tf | 431.83 | K | Joback Method |
| vc | 0.328 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 175.49 | J/mol×K | 492.23 | Joback Method |
| cpg | 185.10 | J/mol×K | 539.97 | Joback Method |
| cpg | 193.71 | J/mol×K | 587.70 | Joback Method |
| cpg | 201.43 | J/mol×K | 635.44 | Joback Method |
| cpg | 208.34 | J/mol×K | 683.17 | Joback Method |
| cpg | 214.54 | J/mol×K | 730.91 | Joback Method |
| cpg | 220.13 | J/mol×K | 778.64 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C252095&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 |
| **ie:** | Ionization energy |
| **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 |