# 1,3-Benzenedimethanethiol, S,S'-diacetyl-

**Inchi:** InChI=1S/C12H14O2S2/c1-9(13)15-7-11-4-3-5-12(6-11)8-16-10(2)14/h3-6H,7-8H2,1-2H
**InchiKey:** CHZGFXFUJVVNRX-UHFFFAOYSA-N
**Formula:** C12H14O2S2
**SMILES:** CC(=O)SCc1cccc(CSC(C)=O)c1
**Mol. weight [g/mol]:** 254.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -38.66 | kJ/mol | Joback Method |
| hf | -207.37 | kJ/mol | Joback Method |
| hfus | 31.95 | kJ/mol | Joback Method |
| hvap | 72.37 | kJ/mol | Joback Method |
| log10ws | -4.22 | | Crippen Method |
| logp | 3.246 | | Crippen Method |
| mcvol | 192.020 | ml/mol | McGowan Method |
| pc | 2787.66 | kPa | Joback Method |
| rinpol | 2055.80 | | NIST Webbook |
| rinpol | 2055.80 | | NIST Webbook |
| tb | 750.92 | K | Joback Method |
| tc | 999.06 | K | Joback Method |
| tf | 432.60 | K | Joback Method |
| vc | 0.720 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 487.72 | J/mol×K | 750.92 | Joback Method |
| cpg | 500.54 | J/mol×K | 792.28 | Joback Method |
| cpg | 512.21 | J/mol×K | 833.63 | Joback Method |
| cpg | 522.76 | J/mol×K | 874.99 | Joback Method |
| cpg | 532.21 | J/mol×K | 916.35 | Joback Method |
| cpg | 540.59 | J/mol×K | 957.70 | Joback Method |
| cpg | 547.92 | J/mol×K | 999.06 | 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=U353030&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |