# 3,5-Heptanedione, 1,7-bis(4-hydroxy-3-methoxyphenyl)-

**Other names:** Tetrahydrodiferuloylmethane
Tetrahydrocurcumin
1,7-bis(4-Hydroxy-3-methoxyphenyl)heptane-3,5-dione

**Inchi:** InChI=1S/C21H24O6/c1-26-20-11-14(5-9-18(20)24)3-7-16(22)13-17(23)8-4-15-6-10-19(2

**InchiKey:** LBTVHXHERHESKG-UHFFFAOYSA-N

**Formula:** C21H24O6

**SMILES:** COc1cc(CCC(=O)CC(=O)CCc2ccc(O)c(OC)c2)ccc1O

**Mol. weight [g/mol]:** 372.41

**CAS:** 36062-04-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -445.58 | kJ/mol | Joback Method |
| hf | -870.87 | kJ/mol | Joback Method |
| hfus | 54.59 | kJ/mol | Joback Method |
| hvap | 112.56 | kJ/mol | Joback Method |
| log10ws | -3.88 | | Crippen Method |
| logp | 3.209 | | Crippen Method |
| mcvol | 285.850 | ml/mol | McGowan Method |
| pc | 2043.76 | kPa | Joback Method |
| rinpol | 3187.60 | | NIST Webbook |
| rinpol | 3187.60 | | NIST Webbook |
| tb | 1057.02 | K | Joback Method |
| tc | 1301.28 | K | Joback Method |
| tf | 772.07 | K | Joback Method |
| vc | 0.976 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 940.89 | J/mol×K | 1057.02 | Joback Method |
| cpg | 955.75 | J/mol×K | 1097.73 | Joback Method |
| cpg | 970.44 | J/mol×K | 1138.44 | Joback Method |
| cpg | 985.09 | J/mol×K | 1179.15 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 999.88 | J/mol×K | 1219.86 | Joback Method |
| cpg | 1014.94 | J/mol×K | 1260.57 | Joback Method |
| cpg | 1030.44 | J/mol×K | 1301.28 | Joback Method |
| dvisc | 0.0000007 | Pa×s | 772.07 | Joback Method |
| dvisc | 0.0000004 | Pa×s | 819.56 | Joback Method |
| dvisc | 0.0000002 | Pa×s | 867.05 | Joback Method |
| dvisc | 0.0000001 | Pa×s | 914.54 | Joback Method |
| dvisc | 8.9906777e-08 | Pa×s | 962.04 | Joback Method |
| dvisc | 6.0756764e-08 | Pa×s | 1009.53 | Joback Method |
| dvisc | 4.2529545e-08 | Pa×s | 1057.02 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C36062041&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
**dvisc:** Dynamic viscosity
**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

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