# Ethanone, 1-(2,4,6-trihydroxyphenyl)-

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|---|---|
| **Other names:** | Acetophenone, 2',4',6'-trihydroxy- |
| | Acetophloroglucine |
| | Acetylphloroglucinol |
| | Phloroacetophenone |
| | 1-(2,4,6-Trihydroxyphenyl)ethanone |
| | 2',4',6'-Trihydroxyacetophenone |
| | 2,4,6-Trihydroxyacetophenone |
| | Phloracetophenone |
| | Phloracetophene |
| | NSC 54927 |
| **Inchi:** | InChI=1S/C8H8O4/c1-4(9)8-6(11)2-5(10)3-7(8)12/h2-3,10-12H,1H3 |
| **InchiKey:** | XLEYFDVVXLMULC-UHFFFAOYSA-N |
| **Formula:** | C8H8O4 |
| **SMILES:** | CC(=O)c1c(O)cc(O)cc1O |
| **Mol. weight [g/mol]:** | 168.15 |
| **CAS:** | 480-66-0 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -463.89 | kJ/mol | Joback Method |
| hf | -616.43 | kJ/mol | Joback Method |
| hfus | 29.46 | kJ/mol | Joback Method |
| hvap | 81.47 | kJ/mol | Joback Method |
| log10ws | -0.78 | | Crippen Method |
| logp | 1.006 | | Crippen Method |
| mcvol | 119.000 | ml/mol | McGowan Method |
| pc | 7627.62 | kPa | Joback Method |
| tb | 704.85 | K | Joback Method |
| tc | 958.07 | K | Joback Method |
| tf | 591.43 | K | Joback Method |
| vc | 0.280 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 314.57 | J/mol×K | 704.85 | Joback Method |
| cpg | 322.12 | J/mol×K | 747.05 | Joback Method |
| cpg | 329.41 | J/mol×K | 789.26 | Joback Method |
| cpg | 336.67 | J/mol×K | 831.46 | Joback Method |
| cpg | 344.12 | J/mol×K | 873.67 | Joback Method |
| cpg | 351.99 | J/mol×K | 915.87 | Joback Method |
| cpg | 360.50 | J/mol×K | 958.07 | Joback Method |
| dvisc | 0.0000027 | Pa×s | 591.43 | Joback Method |
| dvisc | 0.0000017 | Pa×s | 610.33 | Joback Method |
| dvisc | 0.0000011 | Pa×s | 629.24 | Joback Method |
| dvisc | 0.0000007 | Pa×s | 648.14 | Joback Method |
| dvisc | 0.0000005 | Pa×s | 667.04 | Joback Method |
| dvisc | 0.0000003 | Pa×s | 685.95 | Joback Method |
| dvisc | 0.0000002 | Pa×s | 704.85 | Joback Method |

# Sources

**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=C480660&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# 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
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume