

# 2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetrahydroxy-

Other names: 2,3,5,6-Tetrahydroxy-2,5-cyclohexadien-1,4-dione  
2,3,5,6-Tetrahydroxy-p-benzoquinone  
2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetrahydroxy-  
HPEK-1  
Kelox  
NSC-112931  
THQ  
Terasin  
Tetrahydroxy-1,4-benzoquinone  
Tetrahydroxy-1,4-quinone  
Tetrahydroxy-p-benzoquinone  
Tetrahydroxy-p-quinone  
Tetrahydroxyparabenzoquinone  
Tetrahydroxyquinone  
p-Benzoquinone, 2,3,5,6-tetrahydroxy-

Inchi: InChI=1S/C6H4O6/c7-1-2(8)4(10)6(12)5(11)3(1)9/h7-8,11-12H  
InchiKey: DGQOCLATAPFASR-UHFFFAOYSA-N  
Formula: C6H4O6  
SMILES: O=C1C(O)=C(O)C(=O)C(O)=C1O  
Mol. weight [g/mol]: 172.09

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hfus          | 18.32   | kJ/mol | Joback Method  |
| logp          | -0.207  |        | Crippen Method |
| mcvol         | 102.560 | ml/mol | McGowan Method |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 292.83 | J/mol×K | 883.50          | Joback Method |
| cpg           | 297.33 | J/mol×K | 917.68          | Joback Method |
| cpg           | 301.20 | J/mol×K | 951.86          | Joback Method |
| cpg           | 304.38 | J/mol×K | 986.04          | Joback Method |

|     |        |         |         |               |
|-----|--------|---------|---------|---------------|
| cpg | 306.83 | J/mol×K | 1020.22 | Joback Method |
| cpg | 308.51 | J/mol×K | 1054.40 | Joback Method |
| cpg | 309.38 | J/mol×K | 1088.58 | Joback Method |

## Sources

|                                  |                                                                                                                                           |
|----------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C319891&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C319891&amp;Units=SI</a> |
| <b>Joback Method:</b>            | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b>           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>Crippen Method:</b>           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b>           | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                         |
| <b>Cheméo Relay (1.0):</b>       |                                                                                                                                           |
| <b>Cheméo Relay (1.0, beta):</b> |                                                                                                                                           |

## Legend

|               |                                           |
|---------------|-------------------------------------------|
| <b>cpg:</b>   | Ideal gas heat capacity                   |
| <b>hfus:</b>  | Enthalpy of fusion at standard conditions |
| <b>logp:</b>  | Octanol/Water partition coefficient       |
| <b>mcvol:</b> | McGowan's characteristic volume           |

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