

2,5-Cyclohexadiene-1,4-dione, 2,5-bis(4-methoxyphenyl)-

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|----------------------|--|
| Other names: | 2,5-Di-p-anisyl-1,4-benzoquinone |
| Inchi: | InChI=1S/C20H16O4/c1-23-15-7-3-13(4-8-15)17-11-20(22)18(12-19(17)21)14-5-9-16(24 |
| InchiKey: | JZJYUHYPMJANNP-UHFFFAOYSA-N |
| Formula: | C20H16O4 |
| SMILES: | COc1ccc(C2=CC(=O)C(c3ccc(OC)cc3)=CC2=O)cc1 |
| Mol. weight [g/mol]: | 320.34 |
| CAS: | 5333-03-9 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -59.28 | kJ/mol | Joback Method |
| hf | -378.57 | kJ/mol | Joback Method |
| hfus | 28.69 | kJ/mol | Joback Method |
| hvap | 81.95 | kJ/mol | Joback Method |
| log10ws | -4.30 | | Crippen Method |
| logp | 3.323 | | Crippen Method |
| mcvol | 240.560 | ml/mol | McGowan Method |
| pc | 2085.03 | kPa | Joback Method |
| tb | 933.30 | K | Joback Method |
| tc | 1199.07 | K | Joback Method |
| tf | 612.12 | K | Joback Method |
| vc | 0.895 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 735.11 | J/molxK | 933.30 | Joback Method |
| cpg | 747.58 | J/molxK | 977.60 | Joback Method |
| cpg | 757.74 | J/molxK | 1021.89 | Joback Method |
| cpg | 765.55 | J/molxK | 1066.19 | Joback Method |
| cpg | 770.95 | J/molxK | 1110.48 | Joback Method |
| cpg | 773.87 | J/molxK | 1154.78 | Joback Method |
| cpg | 774.27 | J/molxK | 1199.07 | 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=C5333039&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |

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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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