# Phenylmaleic anhydride

| | |
|---|---|
| **Other names:** | 2,5-Furandione, 3-phenyl- |
| | 3-phenyl-2,5-furandione |
| | 3-phenylfuran-2,5-dione |
| **Inchi:** | InChI=1S/C10H6O3/c11-9-6-8(10(12)13-9)7-4-2-1-3-5-7/h1-6H |
| **InchiKey:** | QZYCWJVSPFQUQC-UHFFFAOYSA-N |
| **Formula:** | C10H6O3 |
| **SMILES:** | O=C1C=C(c2ccccc2)C(=O)O1 |
| **Mol. weight [g/mol]:** | 174.15 |
| **CAS:** | 36122-35-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| ea | 1.74 ± 0.04 | eV | NIST Webbook |
| gf | -120.98 | kJ/mol | Joback Method |
| hf | -293.47 | kJ/mol | Joback Method |
| hfus | 16.39 | kJ/mol | Joback Method |
| hvap | 54.65 | kJ/mol | Joback Method |
| log10ws | -1.66 | | Crippen Method |
| logp | 1.153 | | Crippen Method |
| mcvol | 121.850 | ml/mol | McGowan Method |
| pc | 4151.61 | kPa | Joback Method |
| tb | 641.56 | K | Joback Method |
| tc | 913.26 | K | Joback Method |
| tf | 393.35 | K | Thermodynamic properties of phase transitions of phenyl derivatives of maleic anhydride and oxazole |
| vc | 0.451 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 299.40 | J/mol×K | 641.56 | Joback Method |
| cpg | 313.14 | J/mol×K | 686.84 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 325.79 | J/mol×K | 732.13 | Joback Method |
| cpg | 337.32 | J/mol×K | 777.41 | Joback Method |
| cpg | 347.71 | J/mol×K | 822.69 | Joback Method |
| cpg | 356.93 | J/mol×K | 867.98 | Joback Method |
| cpg | 364.93 | J/mol×K | 913.26 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C36122357&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Thermodynamic properties of phase transitions of phenyl derivatives of maleic anhydride and oxazole:** | https://www.doi.org/10.1016/j.jct.2018.12.001 |
| **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 |
| **ea:** | Electron affinity |
| **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 |

Latest version available from:

https://www.chemeo.com/cid/14-341-7/Phenylmaleic-anhydride.pdf

Generated by Cheméo on 2024-10-12 04:54:40.879356382 +0000 UTC m=+3289743.516325631.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.