# 1(3H)-Isobenzofuranone, 3-ethoxy-

**Other names:** Phthalide, 3-ethoxy-
3-Ethoxyphthalide
**Inchi:** InChI=1S/C10H10O3/c1-2-12-10-8-6-4-3-5-7(8)9(11)13-10/h3-6,10H,2H2,1H3
**InchiKey:** VCBNFFOSUGMASJ-UHFFFAOYSA-N
**Formula:** C10H10O3
**SMILES:** CCOC1OC(=O)c2ccccc21
**Mol. weight [g/mol]:** 178.18
**CAS:** 16824-02-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -116.86 | kJ/mol | Joback Method |
| hf | -353.79 | kJ/mol | Joback Method |
| hfus | 22.12 | kJ/mol | Joback Method |
| hvap | 51.87 | kJ/mol | Joback Method |
| log10ws | -2.45 | | Crippen Method |
| logp | 1.892 | | Crippen Method |
| mcvol | 130.450 | ml/mol | McGowan Method |
| pc | 3368.44 | kPa | Joback Method |
| tb | 583.79 | K | Joback Method |
| tc | 817.83 | K | Joback Method |
| tf | 376.36 | K | Joback Method |
| vc | 0.490 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 322.24 | J/mol×K | 583.79 | Joback Method |
| cpg | 336.32 | J/mol×K | 622.80 | Joback Method |
| cpg | 349.55 | J/mol×K | 661.80 | Joback Method |
| cpg | 361.95 | J/mol×K | 700.81 | Joback Method |
| cpg | 373.53 | J/mol×K | 739.82 | Joback Method |
| cpg | 384.30 | J/mol×K | 778.82 | Joback Method |
| cpg | 394.27 | J/mol×K | 817.83 | 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=C16824025&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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|---|---|
| **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 |