# Isophthalic acid, ethyl 2-methoxyethyl ester

**Inchi:** InChI=1S/C13H16O5/c1-3-17-12(14)10-5-4-6-11(9-10)13(15)18-8-7-16-2/h4-6,9H,3,7-8H
**InchiKey:** LSZNLFSHZJKMQP-UHFFFAOYSA-N
**Formula:** C13H16O5
**SMILES:** CCOC(=O)c1cccc(C(=O)OCCOC)c1
**Mol. weight [g/mol]:** 252.26

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -411.48 | kJ/mol | Joback Method |
| hf | -708.41 | kJ/mol | Joback Method |
| hfus | 29.84 | kJ/mol | Joback Method |
| hvap | 68.19 | kJ/mol | Joback Method |
| log10ws | -2.30 | | Crippen Method |
| logp | 1.666 | | Crippen Method |
| mcvol | 191.020 | ml/mol | McGowan Method |
| pc | 2322.54 | kPa | Joback Method |
| rinpol | 1919.00 | | NIST Webbook |
| rinpol | 1919.00 | | NIST Webbook |
| tb | 703.50 | K | Joback Method |
| tc | 910.34 | K | Joback Method |
| tf | 441.76 | K | Joback Method |
| vc | 0.722 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 513.53 | J/mol×K | 703.50 | Joback Method |
| cpg | 573.00 | J/mol×K | 875.86 | Joback Method |
| cpg | 562.86 | J/mol×K | 841.39 | Joback Method |
| cpg | 551.84 | J/mol×K | 806.92 | Joback Method |
| cpg | 539.94 | J/mol×K | 772.45 | Joback Method |
| cpg | 527.16 | J/mol×K | 737.97 | Joback Method |
| cpg | 582.24 | J/mol×K | 910.34 | Joback Method |
| dvisc | 0.0001039 | Pa×s | 703.50 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001299 | Pa×s | 659.88 | Joback Method |
| dvisc | 0.0001676 | Pa×s | 616.25 | Joback Method |
| dvisc | 0.0002248 | Pa×s | 572.63 | Joback Method |
| dvisc | 0.0003164 | Pa×s | 529.01 | Joback Method |
| dvisc | 0.0004738 | Pa×s | 485.38 | Joback Method |
| dvisc | 0.0007681 | Pa×s | 441.76 | 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=U345857&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |