# 2-Ethylbutyric acid, 2,6-dimethoxyphenyl ester

**Inchi:** InChI=1S/C14H20O4/c1-5-10(6-2)14(15)18-13-11(16-3)8-7-9-12(13)17-4/h7-10H,5-6H2,
**InchiKey:** WCHUYKAUFKZTLE-UHFFFAOYSA-N
**Formula:** C14H20O4
**SMILES:** CCC(CC)C(=O)Oc1c(OC)cccc1OC
**Mol. weight [g/mol]:** 252.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -286.21 | kJ/mol | Joback Method |
| hf | -633.22 | kJ/mol | Joback Method |
| hfus | 26.92 | kJ/mol | Joback Method |
| hvap | 63.95 | kJ/mol | Joback Method |
| log10ws | -3.46 | | Crippen Method |
| logp | 3.045 | | Crippen Method |
| mcvol | 203.540 | ml/mol | McGowan Method |
| pc | 1991.21 | kPa | Joback Method |
| rinpol | 1779.00 | | NIST Webbook |
| tb | 677.05 | K | Joback Method |
| tc | 879.11 | K | Joback Method |
| tf | 400.62 | K | Joback Method |
| vc | 0.765 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 548.23 | J/mol×K | 677.05 | Joback Method |
| cpg | 617.84 | J/mol×K | 845.44 | Joback Method |
| cpg | 605.67 | J/mol×K | 811.76 | Joback Method |
| cpg | 592.62 | J/mol×K | 778.08 | Joback Method |
| cpg | 578.68 | J/mol×K | 744.40 | Joback Method |
| cpg | 563.88 | J/mol×K | 710.73 | Joback Method |
| cpg | 629.12 | J/mol×K | 879.11 | Joback Method |
| dvisc | 0.0000850 | Pa×s | 677.05 | Joback Method |
| dvisc | 0.0001079 | Pa×s | 630.98 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001422 | Pa×s | 584.91 | Joback Method |
| dvisc | 0.0001964 | Pa×s | 538.84 | Joback Method |
| dvisc | 0.0002882 | Pa×s | 492.76 | Joback Method |
| dvisc | 0.0004578 | Pa×s | 446.69 | Joback Method |
| dvisc | 0.0008086 | Pa×s | 400.62 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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=U369820&Units=SI |

# Legend

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