# Isovaleric acid, 2,3-dimethylphenyl ester

**Inchi:** InChI=1S/C13H18O2/c1-9(2)8-13(14)15-12-7-5-6-10(3)11(12)4/h5-7,9H,8H2,1-4H3
**InchiKey:** ULGFUZCCSGXVDJ-UHFFFAOYSA-N
**Formula:** C13H18O2
**SMILES:** Cc1cccc(OC(=O)CC(C)C)c1C
**Mol. weight [g/mol]:** 206.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -84.63 | kJ/mol | Joback Method |
| hf | -348.14 | kJ/mol | Joback Method |
| hfus | 21.95 | kJ/mol | Joback Method |
| hvap | 56.90 | kJ/mol | Joback Method |
| log10ws | -3.75 | | Crippen Method |
| logp | 3.255 | | Crippen Method |
| mcvol | 177.710 | ml/mol | McGowan Method |
| pc | 2244.00 | kPa | Joback Method |
| rinpol | 1527.00 | | NIST Webbook |
| tb | 609.33 | K | Joback Method |
| tc | 818.21 | K | Joback Method |
| tf | 344.89 | K | Joback Method |
| vc | 0.673 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 443.11 | J/mol×K | 609.33 | Joback Method |
| cpg | 458.82 | J/mol×K | 644.14 | Joback Method |
| cpg | 473.68 | J/mol×K | 678.96 | Joback Method |
| cpg | 487.72 | J/mol×K | 713.77 | Joback Method |
| cpg | 500.94 | J/mol×K | 748.58 | Joback Method |
| cpg | 513.36 | J/mol×K | 783.39 | Joback Method |
| cpg | 524.99 | J/mol×K | 818.21 | Joback Method |
| dvisc | 0.0015959 | Pa×s | 344.89 | Joback Method |
| dvisc | 0.0008629 | Pa×s | 388.96 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0005288 | Pa×s | 433.04 | Joback Method |
| dvisc | 0.0003547 | Pa×s | 477.11 | Joback Method |
| dvisc | 0.0002546 | Pa×s | 521.18 | Joback Method |
| dvisc | 0.0001924 | Pa×s | 565.26 | Joback Method |
| dvisc | 0.0001514 | Pa×s | 609.33 | 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=U360656&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 |