# 2-phenylethyl levulinate

**Inchi:** InChI=1S/C13H16O3/c1-11(14)7-8-13(15)16-10-9-12-5-3-2-4-6-12/h2-6H,7-10H2,1H3
**InchiKey:** FJEDCBJSNFURKI-UHFFFAOYSA-N
**Formula:** C13H16O3
**SMILES:** CC(=O)CCC(=O)OCCc1ccccc1
**Mol. weight [g/mol]:** 220.26

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -191.85 | kJ/mol | Joback Method |
| hf | -432.50 | kJ/mol | Joback Method |
| hfus | 27.85 | kJ/mol | Joback Method |
| hvap | 62.71 | kJ/mol | Joback Method |
| log10ws | -2.51 | | Crippen Method |
| logp | 2.141 | | Crippen Method |
| mcvol | 179.280 | ml/mol | McGowan Method |
| pc | 2436.25 | kPa | Joback Method |
| ripol | 2617.00 | | NIST Webbook |
| ripol | 2617.00 | | NIST Webbook |
| tb | 653.68 | K | Joback Method |
| tc | 863.60 | K | Joback Method |
| tf | 384.78 | K | Joback Method |
| vc | 0.685 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 462.59 | J/mol×K | 653.68 | Joback Method |
| cpg | 476.96 | J/mol×K | 688.67 | Joback Method |
| cpg | 490.43 | J/mol×K | 723.65 | Joback Method |
| cpg | 503.02 | J/mol×K | 758.64 | Joback Method |
| cpg | 514.76 | J/mol×K | 793.62 | Joback Method |
| cpg | 525.67 | J/mol×K | 828.61 | Joback Method |
| cpg | 535.78 | J/mol×K | 863.60 | Joback Method |
| dvisc | 0.0017744 | Pa×s | 384.78 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0009819 | Pa×s | 429.60 | Joback Method |
| dvisc | 0.0006076 | Pa×s | 474.41 | Joback Method |
| dvisc | 0.0004085 | Pa×s | 519.23 | Joback Method |
| dvisc | 0.0002925 | Pa×s | 564.05 | Joback Method |
| dvisc | 0.0002200 | Pa×s | 608.86 | Joback Method |
| dvisc | 0.0001721 | Pa×s | 653.68 | Joback Method |

# Sources

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|---|---|
| **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=R321398&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |