

# 1,3-Dioxolane, 2-ethyl-4-phenyl, # 2

|                      |   |
|----------------------|---|
| Inchi:               | InChI=1S/C11H14O2/c1-2-11-12-8-10(13-11)9-6-4-3-5-7-9/h3-7,10-11H,2,8H2,1H3 |
| InchiKey:            | YK GKRD IKDN YZNF-UHFFFAOYSA-N  |
| Formula:             | C11H14O2  |
| SMILES:              | CCC1OCC(c2ccccc2)O1   |
| Mol. weight [g/mol]: | 178.23  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 10.75   | kJ/mol  | Joback Method  |
| hf            | -257.70 | kJ/mol  | Joback Method  |
| hfus          | 29.25   | kJ/mol  | Joback Method  |
| hvap          | 51.32   | kJ/mol  | Joback Method  |
| log10ws       | -2.67   |         | Crippen Method |
| logp          | 2.511   |         | Crippen Method |
| mcvol         | 142.970 | ml/mol  | McGowan Method |
| pc            | 3038.96 | kPa     | Joback Method  |
| rinpol        | 1333.00 |         | NIST Webbook   |
| rinpol        | 1333.00 |         | NIST Webbook   |
| ripol         | 1880.00 |         | NIST Webbook   |
| ripol         | 1880.00 |         | NIST Webbook   |
| tb            | 542.27  | K       | Joback Method  |
| tc            | 773.49  | K       | Joback Method  |
| tf            | 299.95  | K       | Joback Method  |
| vc            | 0.525   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 349.88 | J/molxK | 542.27          | Joback Method |
| cpg           | 368.02 | J/molxK | 580.81          | Joback Method |
| cpg           | 384.95 | J/molxK | 619.34          | Joback Method |
| cpg           | 400.72 | J/molxK | 657.88          | Joback Method |
| cpg           | 415.37 | J/molxK | 696.42          | Joback Method |
| cpg           | 428.95 | J/molxK | 734.95          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 441.52    | J/molxK | 773.49 | Joback Method |
| dvisc | 0.0031907 | Paxs    | 299.95 | Joback Method |
| dvisc | 0.0017650 | Paxs    | 340.34 | Joback Method |
| dvisc | 0.0011070 | Paxs    | 380.72 | Joback Method |
| dvisc | 0.0007593 | Paxs    | 421.11 | Joback Method |
| dvisc | 0.0005564 | Paxs    | 461.50 | Joback Method |
| dvisc | 0.0004286 | Paxs    | 501.88 | Joback Method |
| dvisc | 0.0003432 | Paxs    | 542.27 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R409200&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R409200&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>ripol:</b>   | Polar retention indices                         |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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