

# Benzene, 1,3-dimethoxy-5-propyl

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C11H16O2/c1-4-5-9-6-10(12-2)8-11(7-9)13-3/h6-8H,4-5H2,1-3H3 |
| InchiKey:            | UHLXFCGEIFTPSB-UHFFFAOYSA-N  |
| Formula:             | C11H16O2   |
| SMILES:              | CCc1cc(OC)cc(OC)c1   |
| Mol. weight [g/mol]: | 180.24   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -75.11  | kJ/mol               | Joback Method  |
| hf            | -321.22 | kJ/mol               | Joback Method  |
| hfus          | 19.89   | kJ/mol               | Joback Method  |
| hvap          | 48.50   | kJ/mol               | Joback Method  |
| log10ws       | -2.93   |                      | Crippen Method |
| logp          | 2.656   |                      | Crippen Method |
| mvol          | 153.830 | ml/mol               | McGowan Method |
| pc            | 2482.59 | kPa                  | Joback Method  |
| rinpol        | 1411.00 |                      | NIST Webbook   |
| tb            | 532.56  | K                    | Joback Method  |
| tc            | 733.53  | K                    | Joback Method  |
| tf            | 309.65  | K                    | Joback Method  |
| vc            | 0.580   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 351.48    | J/molxK | 532.56          | Joback Method |
| cpg           | 418.55    | J/molxK | 700.03          | Joback Method |
| cpg           | 406.38    | J/molxK | 666.54          | Joback Method |
| cpg           | 393.58    | J/molxK | 633.04          | Joback Method |
| cpg           | 380.17    | J/molxK | 599.55          | Joback Method |
| cpg           | 366.13    | J/molxK | 566.05          | Joback Method |
| cpg           | 430.10    | J/molxK | 733.53          | Joback Method |
| dvisc         | 0.0001437 | Paxs    | 532.56          | Joback Method |
| dvisc         | 0.0001780 | Paxs    | 495.41          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002283 | Paxs | 458.26 | Joback Method |
| dvisc | 0.0003060 | Paxs | 421.10 | Joback Method |
| dvisc | 0.0004340 | Paxs | 383.95 | Joback Method |
| dvisc | 0.0006634 | Paxs | 346.80 | Joback Method |
| dvisc | 0.0011230 | Paxs | 309.65 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R143252&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R143252&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>                                 |
| <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>                     |

## 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>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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