

# BENZENE, 4-ETHYL-1,2-DIMETHOXY-

|                      |                                                                 |
|----------------------|-----------------------------------------------------------------|
| Other names:         | 4-Ethyl-1,2-dimethoxybenzene<br>4-Ethyl-2-methoxyanisole        |
| Inchi:               | InChI=1S/C10H14O2/c1-4-8-5-6-9(11-2)10(7-8)12-3/h5-7H,4H2,1-3H3 |
| InchiKey:            | NEBQMYHKOREVAL-UHFFFAOYSA-N                                     |
| Formula:             | C10H14O2                                                        |
| SMILES:              | CCc1ccc(OC)c(OC)c1                                              |
| Mol. weight [g/mol]: | 166.22                                                          |

## Physical Properties

| Property code | Value   | Unit    | Source             |
|---------------|---------|---------|--------------------|
| af            | 0.5327  |         | Cheméo Relay (1.0) |
| hfus          | 17.29   | kJ/mol  | Joback Method      |
| hvap          | 66.74   | kJ/mol  | Cheméo Relay (1.0) |
| ie            | 7.90    | eV      | Cheméo Relay (1.0) |
| log10ws       | -2.76   |         | Cheméo Relay (1.0) |
| logp          | 2.266   |         | Crippen Method     |
| mcvol         | 139.740 | ml/mol  | McGowan Method     |
| pc            | 2738.28 | kPa     | Joback Method      |
| ripol         | 1875.00 |         | NIST Webbook       |
| ripol         | 1875.00 |         | NIST Webbook       |
| tb            | 504.10  | K       | Cheméo Relay (1.0) |
| tc            | 699.30  | K       | Cheméo Relay (1.0) |
| tf            | 281.09  | K       | Cheméo Relay (1.0) |
| vc            | 0.522   | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 306.17 | J/mol×K | 509.68          | Joback Method |
| cpg           | 319.83 | J/mol×K | 543.66          | Joback Method |
| cpg           | 332.95 | J/mol×K | 577.64          | Joback Method |
| cpg           | 345.51 | J/mol×K | 611.62          | Joback Method |
| cpg           | 357.50 | J/mol×K | 645.60          | Joback Method |
| cpg           | 368.93 | J/mol×K | 679.58          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 379.79    | J/mol×K | 713.56 | Joback Method |
| dvisc | 0.0011096 | Pa×s    | 298.38 | Joback Method |
| dvisc | 0.0006697 | Pa×s    | 333.60 | Joback Method |
| dvisc | 0.0004451 | Pa×s    | 368.81 | Joback Method |
| dvisc | 0.0003177 | Pa×s    | 404.03 | Joback Method |
| dvisc | 0.0002393 | Pa×s    | 439.25 | Joback Method |
| dvisc | 0.0001880 | Pa×s    | 474.46 | Joback Method |
| dvisc | 0.0001528 | Pa×s    | 509.68 | Joback Method |

## Sources

|                                  |                                                                                                                                             |
|----------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5888517&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5888517&amp;Units=SI</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>Crippen Method:</b>           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>Cheméo Relay (1.0):</b>       |                                                                                                                                             |
| <b>Cheméo Relay (1.0, beta):</b> |                                                                                                                                             |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>af:</b>      | Acentric Factor                                 |
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>ie:</b>      | Ionization energy                               |
| <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>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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