

# Carbonic acid, 2-chloroethyl 4-methoxyphenyl ester

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C10H11ClO4/c1-13-8-2-4-9(5-3-8)15-10(12)14-7-6-11/h2-5H,6-7H2,1H3 |
| InchiKey:            | PFYLWBGYOBTSRT-UHFFFAOYSA-N  |
| Formula:             | C10H11ClO4   |
| SMILES:              | COc1ccc(OC(=O)OCCCl)cc1  |
| Mol. weight [g/mol]: | 230.65   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -319.75 | kJ/mol               | Joback Method  |
| hf            | -549.65 | kJ/mol               | Joback Method  |
| hfus          | 24.67   | kJ/mol               | Joback Method  |
| hvap          | 59.15   | kJ/mol               | Joback Method  |
| log10ws       | -2.54   |                      | Crippen Method |
| logp          | 2.449   |                      | Crippen Method |
| mvol          | 159.420 | ml/mol               | McGowan Method |
| pc            | 2808.38 | kPa                  | Joback Method  |
| rinpol        | 1751.00 |                      | NIST Webbook   |
| tb            | 618.42  | K                    | Joback Method  |
| tc            | 831.50  | K                    | Joback Method  |
| tf            | 387.94  | K                    | Joback Method  |
| vc            | 0.597   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 373.06    | J/molxK | 618.42          | Joback Method |
| cpg           | 385.20    | J/molxK | 653.93          | Joback Method |
| cpg           | 396.67    | J/molxK | 689.45          | Joback Method |
| cpg           | 407.47    | J/molxK | 724.96          | Joback Method |
| cpg           | 417.57    | J/molxK | 760.47          | Joback Method |
| cpg           | 426.97    | J/molxK | 795.98          | Joback Method |
| cpg           | 435.64    | J/molxK | 831.50          | Joback Method |
| dvisc         | 0.0009281 | Paxs    | 387.94          | Joback Method |
| dvisc         | 0.0005809 | Paxs    | 426.35          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003928 | Paxs | 464.77 | Joback Method |
| dvisc | 0.0002820 | Paxs | 503.18 | Joback Method |
| dvisc | 0.0002122 | Paxs | 541.59 | Joback Method |
| dvisc | 0.0001658 | Paxs | 580.01 | Joback Method |
| dvisc | 0.0001336 | Paxs | 618.42 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U357887&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357887&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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