

# Carbamic acid, 4-methylphenyl, ethyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C10H13NO2/c1-3-13-10(12)11-9-6-4-8(2)5-7-9/h4-7H,3H2,1-2H3,(H,11,12)

RGLJNFKWUYDVBI-UHFFFAOYSA-N

C10H13NO2

CCOC(=O)Nc1ccc(C)cc1

179.22

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -8.43   | kJ/mol  | Joback Method  |
| hf            | -216.00 | kJ/mol  | Joback Method  |
| hfus          | 23.19   | kJ/mol  | Joback Method  |
| hvap          | 56.38   | kJ/mol  | Joback Method  |
| log10ws       | -2.63   |         | Crippen Method |
| logp          | 2.563   |         | Crippen Method |
| mcvol         | 145.420 | ml/mol  | McGowan Method |
| pc            | 3076.16 | kPa     | Joback Method  |
| rinpol        | 1500.00 |         | NIST Webbook   |
| rinpol        | 1495.00 |         | NIST Webbook   |
| rinpol        | 1496.00 |         | NIST Webbook   |
| tb            | 586.32  | K       | Joback Method  |
| tc            | 800.02  | K       | Joback Method  |
| tf            | 366.22  | K       | Joback Method  |
| vc            | 0.546   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 347.62 | J/mol×K | 586.32          | Joback Method |
| cpg           | 360.93 | J/mol×K | 621.94          | Joback Method |
| cpg           | 373.47 | J/mol×K | 657.55          | Joback Method |
| cpg           | 385.26 | J/mol×K | 693.17          | Joback Method |
| cpg           | 396.32 | J/mol×K | 728.79          | Joback Method |
| cpg           | 406.66 | J/mol×K | 764.40          | Joback Method |
| cpg           | 416.30 | J/mol×K | 800.02          | Joback Method |

# Sources

|                        |                                                                                                                                         |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| <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>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=R37866&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R37866&amp;Units=SI</a> |

# Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <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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