

# Carbonic acid, monoamide, N-isobutyl-, hexyl ester

|                      |   |
|----------------------|---|
| Inchi:               | InChI=1S/C11H23NO2/c1-4-5-6-7-8-14-11(13)12-9-10(2)3/h10H,4-9H2,1-3H3,(H,12,13) |
| InchiKey:            | IZWHBMNOJYZVSK-UHFFFAOYSA-N   |
| Formula:             | C11H23NO2   |
| SMILES:              | CCCCCOC(=O)NCC(C)C  |
| Mol. weight [g/mol]: | 201.31  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -105.23 | kJ/mol               | Joback Method  |
| hf            | -466.98 | kJ/mol               | Joback Method  |
| hfus          | 28.61   | kJ/mol               | Joback Method  |
| hvap          | 55.28   | kJ/mol               | Joback Method  |
| log10ws       | -3.22   |                      | Crippen Method |
| logp          | 2.949   |                      | Crippen Method |
| mvol          | 183.270 | ml/mol               | McGowan Method |
| pc            | 2053.03 | kPa                  | Joback Method  |
| rinpol        | 1478.00 |                      | NIST Webbook   |
| rinpol        | 1478.00 |                      | NIST Webbook   |
| tb            | 577.10  | K                    | Joback Method  |
| tc            | 753.70  | K                    | Joback Method  |
| tf            | 323.55  | K                    | Joback Method  |
| vc            | 0.705   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 470.14 | J/molxK | 577.10          | Joback Method |
| cpg           | 485.47 | J/molxK | 606.53          | Joback Method |
| cpg           | 500.16 | J/molxK | 635.97          | Joback Method |
| cpg           | 514.20 | J/molxK | 665.40          | Joback Method |
| cpg           | 527.61 | J/molxK | 694.84          | Joback Method |
| cpg           | 540.39 | J/molxK | 724.27          | Joback Method |
| cpg           | 552.57 | J/molxK | 753.70          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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=U406777&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406777&amp;Units=SI</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>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>h vap:</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>r in pol:</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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