

# 1-Naphthyl n-propylcarbamate

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C14H15NO2/c1-2-10-15-14(16)17-13-9-5-7-11-6-3-4-8-12(11)13/h3-9H,2,10H2 |
| InchiKey:            | UXYGKIWSDXDEMU-UHFFFAOYSA-N                                                      |
| Formula:             | C14H15NO2                                                                        |
| SMILES:              | CCCN(C(=O)Oc1cccc2ccccc12                                                        |
| Mol. weight [g/mol]: | 229.27                                                                           |
| CAS:                 | 25216-27-7                                                                       |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 131.90  | kJ/mol  | Joback Method  |
| hf            | -107.49 | kJ/mol  | Joback Method  |
| hfus          | 30.57   | kJ/mol  | Joback Method  |
| hvap          | 66.93   | kJ/mol  | Joback Method  |
| log10ws       | -4.59   |         | Crippen Method |
| logp          | 3.338   |         | Crippen Method |
| mcvol         | 182.320 | ml/mol  | McGowan Method |
| pc            | 2651.56 | kPa     | Joback Method  |
| tb            | 696.82  | K       | Joback Method  |
| tc            | 921.37  | K       | Joback Method  |
| tf            | 444.00  | K       | Joback Method  |
| vc            | 0.693   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 485.05 | J/mol×K | 696.82          | Joback Method |
| cpg           | 499.08 | J/mol×K | 734.24          | Joback Method |
| cpg           | 512.12 | J/mol×K | 771.67          | Joback Method |
| cpg           | 524.23 | J/mol×K | 809.09          | Joback Method |
| cpg           | 535.47 | J/mol×K | 846.52          | Joback Method |
| cpg           | 545.89 | J/mol×K | 883.94          | Joback Method |
| cpg           | 555.56 | J/mol×K | 921.37          | Joback Method |

# Sources

|                        |                                                                                                                                               |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=C25216277&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C25216277&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>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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