

# Butyric acid, 2-phenyl-, naphth-2-yl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C20H18O2/c1-2-19(16-9-4-3-5-10-16)20(21)22-18-13-12-15-8-6-7-11-17(15)14

HIHXLDAQNELJQMF-UHFFFAOYSA-N

C20H18O2

CCC(C(=O)Oc1ccc2ccccc2c1)c1ccccc1

290.36

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 203.00  | kJ/mol  | Joback Method  |
| hf            | -53.55  | kJ/mol  | Joback Method  |
| hfus          | 31.53   | kJ/mol  | Joback Method  |
| hvap          | 75.74   | kJ/mol  | Joback Method  |
| log10ws       | -6.01   |         | Crippen Method |
| logp          | 4.939   |         | Crippen Method |
| mcvol         | 233.120 | ml/mol  | McGowan Method |
| pc            | 2081.22 | kPa     | Joback Method  |
| rinpol        | 2480.00 |         | NIST Webbook   |
| rinpol        | 2480.00 |         | NIST Webbook   |
| tb            | 810.17  | K       | Joback Method  |
| tc            | 1055.99 | K       | Joback Method  |
| tf            | 470.38  | K       | Joback Method  |
| vc            | 0.879   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 666.42    | J/mol×K | 810.17          | Joback Method |
| cpg           | 681.93    | J/mol×K | 851.14          | Joback Method |
| cpg           | 696.16    | J/mol×K | 892.11          | Joback Method |
| cpg           | 709.22    | J/mol×K | 933.08          | Joback Method |
| cpg           | 721.22    | J/mol×K | 974.05          | Joback Method |
| cpg           | 732.28    | J/mol×K | 1015.02         | Joback Method |
| cpg           | 742.51    | J/mol×K | 1055.99         | Joback Method |
| dvisc         | 0.0010632 | Pa×s    | 470.38          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0006261 | Pa×s | 527.01 | Joback Method |
| dvisc | 0.0004086 | Pa×s | 583.64 | Joback Method |
| dvisc | 0.0002876 | Pa×s | 640.27 | Joback Method |
| dvisc | 0.0002143 | Pa×s | 696.91 | Joback Method |
| dvisc | 0.0001669 | Pa×s | 753.54 | Joback Method |
| dvisc | 0.0001346 | Pa×s | 810.17 | 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=U406876&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406876&amp;Units=SI</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                                 |

Latest version available from:

<https://www.chemeo.com/cid/80-632-1/Butyric-acid-2-phenyl-naphth-2-yl-ester.pdf>

Generated by Cheméo on 2025-12-21 21:29:07.24535652 +0000 UTC m=+6100744.775397174.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.