

# 3-Cyclopentylpropionic acid, 2-naphthyl ester

**Inchi:** InChI=1S/C18H20O2/c19-18(12-9-14-5-1-2-6-14)20-17-11-10-15-7-3-4-8-16(15)13-17/h3-18,20-21H,1H2  
**InchiKey:** AWDSCFKWFOHGC-UHFFFAOYSA-N  
**Formula:** C18H20O2  
**SMILES:** O=C(CCC1CCCC1)Oc1ccc2ccccc2c1  
**Mol. weight [g/mol]:** 268.35

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 112.74  | kJ/mol  | Joback Method  |
| hf            | -183.04 | kJ/mol  | Joback Method  |
| hfus          | 29.77   | kJ/mol  | Joback Method  |
| hvap          | 69.65   | kJ/mol  | Joback Method  |
| log10ws       | -5.75   |         | Crippen Method |
| logp          | 4.716   |         | Crippen Method |
| mcvol         | 217.840 | ml/mol  | McGowan Method |
| pc            | 2145.33 | kPa     | Joback Method  |
| rinpol        | 2298.00 |         | NIST Webbook   |
| tb            | 753.45  | K       | Joback Method  |
| tc            | 990.80  | K       | Joback Method  |
| tf            | 447.32  | K       | Joback Method  |
| vc            | 0.823   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 635.60    | J/mol×K | 753.45          | Joback Method |
| cpg           | 653.37    | J/mol×K | 793.01          | Joback Method |
| cpg           | 669.79    | J/mol×K | 832.57          | Joback Method |
| cpg           | 684.94    | J/mol×K | 872.12          | Joback Method |
| cpg           | 698.93    | J/mol×K | 911.68          | Joback Method |
| cpg           | 711.84    | J/mol×K | 951.24          | Joback Method |
| cpg           | 723.78    | J/mol×K | 990.80          | Joback Method |
| dvisc         | 0.0015637 | Pa×s    | 447.32          | Joback Method |
| dvisc         | 0.0009964 | Pa×s    | 498.34          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0006903 | Pa×s | 549.36 | Joback Method |
| dvisc | 0.0005091 | Pa×s | 600.38 | Joback Method |
| dvisc | 0.0003937 | Pa×s | 651.41 | Joback Method |
| dvisc | 0.0003161 | Pa×s | 702.43 | Joback Method |
| dvisc | 0.0002615 | Pa×s | 753.45 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U307137&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307137&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>                                     |
| <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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