

# Dicyclohexyl phthalate

|                      |                                                                                                                                                                                                                                                                                                                                             |
|----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 1,2-Benzenedicarboxylic acid, dicyclohexyl ester<br>Phthalic acid, dicyclohexyl ester<br>Ergoplast FDC<br>HF 191<br>KP 201<br>Unimoll 66<br>Ergoplast.fdc<br>Howflex CP<br>DCHP<br>Dicyclohexyl benzene-1,2-dicarboxylate<br>Morflex 150<br>Unimoll 66 M<br>Uniplex 250<br>1,2-Benzenedicarboxylic acid, 1,2-dicyclohexyl ester<br>NSC 6101 |
| Inchi:               | InChI=1S/C20H26O4/c21-19(23-15-9-3-1-4-10-15)17-13-7-8-14-18(17)20(22)24-16-11-5                                                                                                                                                                                                                                                            |
| InchiKey:            | VOWAEIGWURALJQ-UHFFFAOYSA-N                                                                                                                                                                                                                                                                                                                 |
| Formula:             | C20H26O4                                                                                                                                                                                                                                                                                                                                    |
| SMILES:              | O=C(OC1CCCCC1)c1cccc1C(=O)OC1CCCCC1                                                                                                                                                                                                                                                                                                         |
| Mol. weight [g/mol]: | 330.42                                                                                                                                                                                                                                                                                                                                      |
| CAS:                 | 84-61-7                                                                                                                                                                                                                                                                                                                                     |

## Physical Properties

| Property code | Value             | Unit   | Source         |
|---------------|-------------------|--------|----------------|
| chs           | -10655.00 ± 11.00 | kJ/mol | NIST Webbook   |
| gf            | -198.64           | kJ/mol | Joback Method  |
| hf            | -612.03           | kJ/mol | Joback Method  |
| hfs           | -931.00 ± 11.00   | kJ/mol | NIST Webbook   |
| hfus          | 30.45             | kJ/mol | Joback Method  |
| hvap          | 82.22             | kJ/mol | Joback Method  |
| log10ws       | -6.16             |        | Crippen Method |
| logp          | 4.666             |        | Crippen Method |
| mcvol         | 262.060           | ml/mol | McGowan Method |
| pc            | 1857.91           | kPa    | Joback Method  |
| rinpol        | 2475.00           |        | NIST Webbook   |
| rinpol        | 2461.00           |        | NIST Webbook   |
| rinpol        | 2453.00           |        | NIST Webbook   |

|        |         |                      |               |
|--------|---------|----------------------|---------------|
| rinpol | 2472.00 |                      | NIST Webbook  |
| rinpol | 2461.00 |                      | NIST Webbook  |
| rinpol | 2472.00 |                      | NIST Webbook  |
| rinpol | 2523.00 |                      | NIST Webbook  |
| rinpol | 2524.00 |                      | NIST Webbook  |
| rinpol | 2524.00 |                      | NIST Webbook  |
| rinpol | 2526.00 |                      | NIST Webbook  |
| rinpol | 2526.00 |                      | NIST Webbook  |
| rinpol | 2527.00 |                      | NIST Webbook  |
| rinpol | 2533.00 |                      | NIST Webbook  |
| tb     | 880.34  | K                    | Joback Method |
| tc     | 1126.04 | K                    | Joback Method |
| tf     | 513.18  | K                    | Joback Method |
| vc     | 0.962   | m <sup>3</sup> /kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 867.81    | J/mol×K | 880.34          | Joback Method |
| cpg           | 885.81    | J/mol×K | 921.29          | Joback Method |
| cpg           | 901.78    | J/mol×K | 962.24          | Joback Method |
| cpg           | 915.79    | J/mol×K | 1003.19         | Joback Method |
| cpg           | 927.88    | J/mol×K | 1044.14         | Joback Method |
| cpg           | 938.09    | J/mol×K | 1085.09         | Joback Method |
| cpg           | 946.48    | J/mol×K | 1126.04         | Joback Method |
| dvisc         | 0.0007646 | Pa×s    | 513.18          | Joback Method |
| dvisc         | 0.0003967 | Pa×s    | 574.37          | Joback Method |
| dvisc         | 0.0002335 | Pa×s    | 635.57          | Joback Method |
| dvisc         | 0.0001509 | Pa×s    | 696.76          | Joback Method |
| dvisc         | 0.0001046 | Pa×s    | 757.95          | Joback Method |
| dvisc         | 0.0000766 | Pa×s    | 819.15          | Joback Method |
| dvisc         | 0.0000586 | Pa×s    | 880.34          | Joback Method |
| hvapt         | 97.00     | kJ/mol  | 433.00          | NIST Webbook  |

## Sources

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C84617&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

|                 |                                                          |
|-----------------|----------------------------------------------------------|
| <b>chs:</b>     | Standard solid enthalpy of combustion                    |
| <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>hfs:</b>     | Solid phase 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>hvapt:</b>   | Enthalpy of vaporization at a given temperature          |
| <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>rinpola:</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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