# DODECANOIC ACID, PHENYLMETHYL ESTER

**Other names:** Lauric acid, benzyl ester
Benzyl dodecanoate
Benzyl laurate
Dodecanoic acid, benzyl ester
**Inchi:** InChI=1S/C19H30O2/c1-2-3-4-5-6-7-8-9-13-16-19(20)21-17-18-14-11-10-12-15-18/h10-1
**InchiKey:** QNRYOQRUGRVBRL-UHFFFAOYSA-N
**Formula:** C19H30O2
**SMILES:** CCCCCCCCCCCC(=O)OCc1ccccc1
**Mol. weight [g/mol]:** 290.45

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.8693 | | Cheméo Relay (1.0) |
| gf | -12.41 | kJ/mol | Joback Method |
| hf | -488.23 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 41.79 | kJ/mol | Joback Method |
| hvap | 91.02 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.94 | eV | Cheméo Relay (1.0) |
| log10ws | -5.93 | | Cheméo Relay (1.0) |
| logp | 5.651 | | Crippen Method |
| mcvol | 262.250 | ml/mol | McGowan Method |
| pc | 1408.01 | kPa | Joback Method |
| rinpol | 2097.00 | | NIST Webbook |
| rinpol | 2097.00 | | NIST Webbook |
| tb | 604.59 | K | Cheméo Relay (1.0) |
| tc | 809.06 | K | Cheméo Relay (1.0) |
| tf | 280.71 | K | Cheméo Relay (1.0) |
| vc | 0.995 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 768.05 | J/mol×K | 737.09 | Joback Method |
| cpg | 786.09 | J/mol×K | 768.93 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 803.11 | J/mol×K | 800.76 | Joback Method |
| cpg | 819.14 | J/mol×K | 832.60 | Joback Method |
| cpg | 834.22 | J/mol×K | 864.43 | Joback Method |
| cpg | 848.38 | J/mol×K | 896.27 | Joback Method |
| cpg | 861.65 | J/mol×K | 928.11 | Joback Method |
| dvisc | 0.0014187 | Pa×s | 402.47 | Joback Method |
| dvisc | 0.0006659 | Pa×s | 458.24 | Joback Method |
| dvisc | 0.0003683 | Pa×s | 514.01 | Joback Method |
| dvisc | 0.0002288 | Pa×s | 569.78 | Joback Method |
| dvisc | 0.0001547 | Pa×s | 625.55 | Joback Method |
| dvisc | 0.0001115 | Pa×s | 681.32 | Joback Method |
| dvisc | 0.0000845 | Pa×s | 737.09 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Cheméo Relay (1.0):**
**Cheméo Relay (1.0, beta):**
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C140250&Units=SI
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

# Legend

**af:** Acentric Factor
**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**gf:** Standard Gibbs free energy of formation
**hf:** Enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hvap:** Enthalpy of vaporization at standard conditions
**ie:** Ionization energy
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**pc:** Critical Pressure
**rinpol:** Non-polar retention indices

| | |
|---|---|
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |