

Butyric acid, 2-phenyl-, dec-2-yl ester

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|-----------------------------|-----------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C20H32O2/c1-4-6-7-8-9-11-14-17(3)22-20(21)19(5-2)18-15-12-10-13-16-18/h1 |
| InchiKey: | YCJYBWZDPUJMEG-UHFFFAOYSA-N |
| Formula: | C20H32O2 |
| SMILES: | CCCCCCCC(C)OC(=O)C(CC)c1ccccc1 |
| Mol. weight [g/mol]: | 304.47 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -8.87 | kJ/mol | Joback Method |
| hf | -474.96 | kJ/mol | Joback Method |
| hfus | 37.34 | kJ/mol | Joback Method |
| hvap | 70.77 | kJ/mol | Joback Method |
| log10ws | -6.24 | | Crippen Method |
| logp | 5.863 | | Crippen Method |
| mvol | 276.340 | ml/mol | McGowan Method |
| pc | 1327.14 | kPa | Joback Method |
| rinpol | 2007.00 | | NIST Webbook |
| tb | 759.09 | K | Joback Method |
| tc | 954.28 | K | Joback Method |
| tf | 383.74 | K | Joback Method |
| vc | 1.060 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 827.19 | J/molxK | 759.09 | Joback Method |
| cpg | 845.94 | J/molxK | 791.62 | Joback Method |
| cpg | 863.57 | J/molxK | 824.15 | Joback Method |
| cpg | 880.12 | J/molxK | 856.68 | Joback Method |
| cpg | 895.64 | J/molxK | 889.21 | Joback Method |
| cpg | 910.15 | J/molxK | 921.75 | Joback Method |
| cpg | 923.71 | J/molxK | 954.28 | Joback Method |
| dvisc | 0.0019655 | Paxs | 383.74 | Joback Method |
| dvisc | 0.0007409 | Paxs | 446.30 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003550 | Paxs | 508.86 | Joback Method |
| dvisc | 0.0001998 | Paxs | 571.41 | Joback Method |
| dvisc | 0.0001260 | Paxs | 633.97 | Joback Method |
| dvisc | 0.0000863 | Paxs | 696.53 | Joback Method |
| dvisc | 0.0000629 | Paxs | 759.09 | Joback Method |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| 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=U406864&Units=SI |

Legend

| | |
|-----------------|-------------------------------------------------|
| 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 |
| 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 |

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<https://www.chemeo.com/cid/87-625-2/Butyric-acid-2-phenyl-dec-2-yl-ester.pdf>

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