

Isophthalic acid, isobutyl oct-3-en-2-yl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C20H28O4/c1-5-6-7-8-10-16(4)24-20(22)18-12-9-11-17(13-18)19(21)23-14-15 |
| InchiKey: | DVEQFNVJVIDLMF-CSKARUKUSA-N |
| Formula: | C20H28O4 |
| SMILES: | CCCCC=CC(C)OC(=O)c1cccc(C(=O)OCC(C)C)c1 |
| Mol. weight [g/mol]: | 332.43 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -172.20 | kJ/mol | Joback Method |
| hf | -614.01 | kJ/mol | Joback Method |
| hfus | 39.94 | kJ/mol | Joback Method |
| hvap | 80.55 | kJ/mol | Joback Method |
| log10ws | -5.87 | | Crippen Method |
| logp | 4.791 | | Crippen Method |
| mvol | 279.480 | ml/mol | McGowan Method |
| pc | 1411.18 | kPa | Joback Method |
| rinpol | 2379.00 | | NIST Webbook |
| rinpol | 2379.00 | | NIST Webbook |
| tb | 844.52 | K | Joback Method |
| tc | 1052.77 | K | Joback Method |
| tf | 463.34 | K | Joback Method |
| vc | 1.063 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 852.32 | J/molxK | 844.52 | Joback Method |
| cpg | 921.03 | J/molxK | 1018.06 | Joback Method |
| cpg | 909.42 | J/molxK | 983.35 | Joback Method |
| cpg | 896.78 | J/molxK | 948.64 | Joback Method |
| cpg | 883.08 | J/molxK | 913.94 | Joback Method |
| cpg | 868.27 | J/molxK | 879.23 | Joback Method |
| cpg | 931.64 | J/molxK | 1052.77 | Joback Method |
| dvisc | 0.0000401 | Paxs | 844.52 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000534 | Paxs | 780.99 | Joback Method |
| dvisc | 0.0000747 | Paxs | 717.46 | Joback Method |
| dvisc | 0.0001116 | Paxs | 653.93 | Joback Method |
| dvisc | 0.0001818 | Paxs | 590.40 | Joback Method |
| dvisc | 0.0003330 | Paxs | 526.87 | Joback Method |
| dvisc | 0.0007202 | Paxs | 463.34 | 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=U343891&Units=SI |

Legend

| | |
|----------------------------|---|
| cp_g: | 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: | Log ₁₀ 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/87-473-1/Isophthalic-acid-isobutyl-oct-3-en-2-yl-ester.pdf>

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