

Formic acid, 2,4-dimethylpent-3-yl ester

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| Inchi: | InChI=1S/C8H16O2/c1-6(2)8(7(3)4)10-5-9/h5-8H,1-4H3 |
| InchiKey: | BATCZJUOZNYSLU-UHFFFAOYSA-N |
| Formula: | C8H16O2 |
| SMILES: | CC(C)C(OC=O)C(C)C |
| Mol. weight [g/mol]: | 144.21 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -195.36 | kJ/mol | Joback Method |
| hf | -442.09 | kJ/mol | Joback Method |
| hfus | 9.38 | kJ/mol | Joback Method |
| hvap | 41.37 | kJ/mol | Joback Method |
| log10ws | -1.66 | | Crippen Method |
| logp | 1.840 | | Crippen Method |
| mvol | 131.020 | ml/mol | McGowan Method |
| pc | 2755.56 | kPa | Joback Method |
| rinpol | 975.00 | | NIST Webbook |
| tb | 452.20 | K | Joback Method |
| tc | 634.23 | K | Joback Method |
| tf | 199.15 | K | Joback Method |
| vc | 0.500 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 281.20 | J/molxK | 452.20 | Joback Method |
| cpg | 294.14 | J/molxK | 482.54 | Joback Method |
| cpg | 306.58 | J/molxK | 512.88 | Joback Method |
| cpg | 318.55 | J/molxK | 543.21 | Joback Method |
| cpg | 330.03 | J/molxK | 573.55 | Joback Method |
| cpg | 341.03 | J/molxK | 603.89 | Joback Method |
| cpg | 351.56 | J/molxK | 634.23 | Joback Method |
| dvisc | 0.0157115 | Paxs | 199.15 | Joback Method |
| dvisc | 0.0042426 | Paxs | 241.32 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0016913 | Paxs | 283.50 | Joback Method |
| dvisc | 0.0008556 | Paxs | 325.68 | Joback Method |
| dvisc | 0.0005060 | Paxs | 367.85 | Joback Method |
| dvisc | 0.0003334 | Paxs | 410.02 | Joback Method |
| dvisc | 0.0002375 | Paxs | 452.20 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=U368261&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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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