

Pentanoic acid, 3-phenylpropyl ester

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| Other names: | Valeric acid, 3-phenylpropyl ester 3-phenylpropyl valerate |
| Inchi: | InChI=1S/C14H20O2/c1-2-3-11-14(15)16-12-7-10-13-8-5-4-6-9-13/h4-6,8-9H,2-3,7,10-12H |
| InchiKey: | OKFJJLRWQHMYCM-UHFFFAOYSA-N |
| Formula: | C14H20O2 |
| SMILES: | CCCCC(=O)OCCc1ccccc1 |
| Mol. weight [g/mol]: | 220.31 |
| CAS: | 5451-88-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -54.51 | kJ/mol | Joback Method |
| hf | -340.56 | kJ/mol | Joback Method |
| hfus | 28.84 | kJ/mol | Joback Method |
| hvap | 58.19 | kJ/mol | Joback Method |
| log10ws | -3.65 | | Crippen Method |
| logp | 3.353 | | Crippen Method |
| mcvol | 191.800 | ml/mol | McGowan Method |
| pc | 2094.58 | kPa | Joback Method |
| rinpola | 1635.00 | | NIST Webbook |
| ripola | 2183.00 | | NIST Webbook |
| ripola | 2183.00 | | NIST Webbook |
| tb | 622.69 | K | Joback Method |
| tc | 822.76 | K | Joback Method |
| tf | 346.12 | K | Joback Method |
| vc | 0.736 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 494.13 | J/molxK | 622.69 | Joback Method |
| cpg | 566.96 | J/molxK | 789.42 | Joback Method |
| cpg | 554.11 | J/molxK | 756.07 | Joback Method |
| cpg | 540.43 | J/molxK | 722.73 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 525.89 | J/molxK | 689.38 | Joback Method |
| cpg | 510.47 | J/molxK | 656.04 | Joback Method |
| cpg | 579.01 | J/molxK | 822.76 | Joback Method |
| dvisc | 0.0001517 | Paxs | 622.69 | Joback Method |
| dvisc | 0.0001969 | Paxs | 576.60 | Joback Method |
| dvisc | 0.0002674 | Paxs | 530.50 | Joback Method |
| dvisc | 0.0003849 | Paxs | 484.40 | Joback Method |
| dvisc | 0.0005982 | Paxs | 438.31 | Joback Method |
| dvisc | 0.0010310 | Paxs | 392.21 | Joback Method |
| dvisc | 0.0020543 | Paxs | 346.12 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C5451887&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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 |
| ripol: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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