

Hex-3-enyl benzoate

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| Other names: | 3-Hexen-1-ol, benzoate 3-Hexenyl-benzoate |
| Inchi: | InChI=1S/C13H16O2/c1-2-3-4-8-11-15-13(14)12-9-6-5-7-10-12/h3-7,9-10H,2,8,11H2,1H |
| InchiKey: | BCOXBEHFBZOJJZ-UHFFFAOYSA-N |
| Formula: | C13H16O2 |
| SMILES: | CCC=CCCOC(=O)c1ccccc1 |
| Mol. weight [g/mol]: | 204.26 |
| CAS: | 72200-74-9 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 17.29 | kJ/mol | Joback Method |
| hf | -202.70 | kJ/mol | Joback Method |
| hfus | 26.46 | kJ/mol | Joback Method |
| hvap | 55.92 | kJ/mol | Joback Method |
| log10ws | -3.66 | | Crippen Method |
| logp | 3.200 | | Crippen Method |
| mcvol | 173.410 | ml/mol | McGowan Method |
| pc | 2410.00 | kPa | Joback Method |
| rinpol | 1573.00 | | NIST Webbook |
| rinpol | 1570.00 | | NIST Webbook |
| rinpol | 1572.60 | | NIST Webbook |
| rinpol | 1579.00 | | NIST Webbook |
| rinpol | 1549.00 | | NIST Webbook |
| rinpol | 1572.60 | | NIST Webbook |
| rinpol | 1546.00 | | NIST Webbook |
| rinpol | 1570.00 | | NIST Webbook |
| rinpol | 1571.00 | | NIST Webbook |
| rinpol | 1571.00 | | NIST Webbook |
| rinpol | 1555.00 | | NIST Webbook |
| ripol | 2065.00 | | NIST Webbook |
| ripol | 2099.00 | | NIST Webbook |
| ripol | 2099.00 | | NIST Webbook |
| tb | 603.97 | K | Joback Method |
| tc | 815.36 | K | Joback Method |
| tf | 329.77 | K | Joback Method |
| vc | 0.659 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 423.08 | J/molxK | 603.97 | Joback Method |
| cpg | 490.65 | J/molxK | 780.13 | Joback Method |
| cpg | 478.84 | J/molxK | 744.90 | Joback Method |
| cpg | 466.22 | J/molxK | 709.66 | Joback Method |
| cpg | 452.75 | J/molxK | 674.43 | Joback Method |
| cpg | 438.38 | J/molxK | 639.20 | Joback Method |
| cpg | 501.68 | J/molxK | 815.36 | Joback Method |
| dvisc | 0.0001434 | Paxs | 603.97 | Joback Method |
| dvisc | 0.0001858 | Paxs | 558.27 | Joback Method |
| dvisc | 0.0002522 | Paxs | 512.57 | Joback Method |
| dvisc | 0.0003633 | Paxs | 466.87 | Joback Method |
| dvisc | 0.0005667 | Paxs | 421.17 | Joback Method |
| dvisc | 0.0009848 | Paxs | 375.47 | Joback Method |
| dvisc | 0.0019948 | Paxs | 329.77 | 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=C72200749&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 |

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