

2«beta»-acetoxy-trans-decalin

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|-----------------------------|--|
| Inchi: | InChI=1S/C12H20O2/c1-9(13)14-12-7-6-10-4-2-3-5-11(10)8-12/h10-12H,2-8H2,1H3/t10? |
| InchiKey: | XKCLIFLFEJJSOAT-HTAVTVPLSA-N |
| Formula: | C12H20O2 |
| SMILES: | CC(=O)OC1CCC2CCCCC2C1 |
| Mol. weight [g/mol]: | 196.29 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -118.37 | kJ/mol | Joback Method |
| hf | -435.19 | kJ/mol | Joback Method |
| hfus | 18.56 | kJ/mol | Joback Method |
| hvap | 51.67 | kJ/mol | Joback Method |
| log10ws | -3.13 | | Crippen Method |
| logp | 2.908 | | Crippen Method |
| mvol | 165.660 | ml/mol | McGowan Method |
| pc | 2507.52 | kPa | Joback Method |
| rinpol | 1429.00 | | NIST Webbook |
| ripol | 1903.00 | | NIST Webbook |
| tb | 576.14 | K | Joback Method |
| tc | 797.36 | K | Joback Method |
| tf | 314.72 | K | Joback Method |
| vc | 0.613 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 443.50 | J/molxK | 576.14 | Joback Method |
| cpg | 538.53 | J/molxK | 760.49 | Joback Method |
| cpg | 522.00 | J/molxK | 723.62 | Joback Method |
| cpg | 504.26 | J/molxK | 686.75 | Joback Method |
| cpg | 485.29 | J/molxK | 649.88 | Joback Method |
| cpg | 465.05 | J/molxK | 613.01 | Joback Method |
| cpg | 553.90 | J/molxK | 797.36 | Joback Method |
| dvisc | 0.0004055 | Paxs | 576.14 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0004935 | Paxs | 532.57 | Joback Method |
| dvisc | 0.0006219 | Paxs | 489.00 | Joback Method |
| dvisc | 0.0008201 | Paxs | 445.43 | Joback Method |
| dvisc | 0.0011482 | Paxs | 401.86 | Joback Method |
| dvisc | 0.0017448 | Paxs | 358.29 | Joback Method |
| dvisc | 0.0029771 | Paxs | 314.72 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R136175&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

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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