

dodec-2-en-4-one

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|-----------------------------|--|
| Inchi: | InChI=1S/C12H22O/c1-3-5-6-7-8-9-11-12(13)10-4-2/h4,10H,3,5-9,11H2,1-2H3/b10-4+ |
| InchiKey: | RBDKOLXWSXOZLC-ONNFQVAWSA-N |
| Formula: | C12H22O |
| SMILES: | CC=CC(=O)CCCCCCCC |
| Mol. weight [g/mol]: | 182.30 |
| CAS: | 65570-26-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 1.46 | kJ/mol | Joback Method |
| hf | -286.37 | kJ/mol | Joback Method |
| hfus | 28.64 | kJ/mol | Joback Method |
| hvap | 49.01 | kJ/mol | Joback Method |
| log10ws | -3.98 | | Crippen Method |
| logp | 3.882 | | Crippen Method |
| mvol | 177.210 | ml/mol | McGowan Method |
| pc | 1966.56 | kPa | Joback Method |
| ripol | 1905.00 | | NIST Webbook |
| tb | 531.99 | K | Joback Method |
| tc | 709.19 | K | Joback Method |
| tf | 269.85 | K | Joback Method |
| vc | 0.694 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 418.56 | J/molxK | 531.99 | Joback Method |
| cpg | 434.19 | J/molxK | 561.52 | Joback Method |
| cpg | 449.11 | J/molxK | 591.06 | Joback Method |
| cpg | 463.35 | J/molxK | 620.59 | Joback Method |
| cpg | 476.93 | J/molxK | 650.12 | Joback Method |
| cpg | 489.87 | J/molxK | 679.66 | Joback Method |
| cpg | 502.21 | J/molxK | 709.19 | Joback Method |
| dvisc | 0.0040892 | Paxs | 269.85 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0017328 | Paxs | 313.54 | Joback Method |
| dvisc | 0.0009059 | Paxs | 357.23 | Joback Method |
| dvisc | 0.0005455 | Paxs | 400.92 | Joback Method |
| dvisc | 0.0003629 | Paxs | 444.61 | Joback Method |
| dvisc | 0.0002597 | Paxs | 488.30 | Joback Method |
| dvisc | 0.0001963 | Paxs | 531.99 | 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=C65570265&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 |
| ripol: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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