

2,4-Heptadienal

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|-----------------------------|---|
| Other names: | hepta-2,4-dienal 2,4-Heptadienal, (Z,Z)- 2,4-Heptadienal, # 2 2,4-Heptandienal |
| Inchi: | InChI=1S/C7H10O/c1-2-3-4-5-6-7-8/h3-7H,2H2,1H3 |
| InchiKey: | SATICYYAWWYRAM-UHFFFAOYSA-N |
| Formula: | C7H10O |
| SMILES: | CCC=CC=CC=O |
| Mol. weight [g/mol]: | 110.15 |
| CAS: | 5910-85-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| gf | 68.98 | kJ/mol | Joback Method |
| hf | -38.95 | kJ/mol | Joback Method |
| hfus | 16.58 | kJ/mol | Joback Method |
| hvap | 37.81 | kJ/mol | Joback Method |
| log10ws | -1.74 | | Crippen Method |
| logp | 1.708 | | Crippen Method |
| mcvol | 102.460 | ml/mol | McGowan Method |
| pc | 3411.87 | kPa | Joback Method |
| rinpol | 965.00 | | NIST Webbook |
| rinpol | 1012.00 | | NIST Webbook |
| rinpol | 982.00 | | NIST Webbook |
| rinpol | 973.00 | | NIST Webbook |
| rinpol | 969.00 | | NIST Webbook |
| rinpol | 1009.00 | | NIST Webbook |
| rinpol | 997.00 | | NIST Webbook |
| rinpol | 955.00 | | NIST Webbook |
| rinpol | 983.00 | | NIST Webbook |
| rinpol | 1012.00 | | NIST Webbook |
| rinpol | 999.00 | | NIST Webbook |
| rinpol | 1013.00 | | NIST Webbook |
| rinpol | 1000.00 | | NIST Webbook |
| rinpol | 998.00 | | NIST Webbook |
| rinpol | 982.00 | | NIST Webbook |
| rinpol | 967.00 | | NIST Webbook |

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| rinpol | 1005.00 | NIST Webbook |
| rinpol | 973.00 | NIST Webbook |
| rinpol | 979.00 | NIST Webbook |
| rinpol | 981.00 | NIST Webbook |
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| rinpol | 966.00 | NIST Webbook |
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| rinpol | 993.00 | NIST Webbook |
| rinpol | 966.00 | NIST Webbook |
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| rinpol | 992.00 | NIST Webbook |
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| rinpol | 987.00 | NIST Webbook |
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| rinpol | 1009.00 | NIST Webbook |
| rinpol | 1030.00 | NIST Webbook |
| rinpol | 996.00 | NIST Webbook |
| rinpol | 1000.00 | NIST Webbook |
| rinpol | 1000.00 | NIST Webbook |
| rinpol | 999.00 | NIST Webbook |
| rinpol | 1000.00 | NIST Webbook |
| rinpol | 958.00 | NIST Webbook |
| rinpol | 997.00 | NIST Webbook |
| rinpol | 1006.00 | NIST Webbook |
| rinpol | 989.00 | NIST Webbook |
| rinpol | 1010.00 | NIST Webbook |
| rinpol | 968.00 | NIST Webbook |
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| ripol | 1503.00 | NIST Webbook |

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| ripol | 1491.00 | | NIST Webbook |
| ripol | 1503.00 | | NIST Webbook |
| ripol | 1510.00 | | NIST Webbook |
| ripol | 1491.00 | | NIST Webbook |
| ripol | 1486.00 | | NIST Webbook |
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| ripol | 1529.00 | | NIST Webbook |
| ripol | 1451.00 | | NIST Webbook |
| ripol | 1489.00 | | NIST Webbook |
| tb | 416.54 | K | Joback Method |
| tc | 606.14 | K | Joback Method |
| tf | 200.49 | K | Joback Method |
| vc | 0.405 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 186.30 | J/molxK | 416.54 | Joback Method |
| cpg | 196.67 | J/molxK | 448.14 | Joback Method |
| cpg | 206.45 | J/molxK | 479.74 | Joback Method |
| cpg | 215.67 | J/molxK | 511.34 | Joback Method |
| cpg | 224.36 | J/molxK | 542.94 | Joback Method |
| cpg | 232.55 | J/molxK | 574.54 | Joback Method |
| cpg | 240.28 | J/molxK | 606.14 | Joback Method |
| dvisc | 0.0039290 | Paxs | 200.49 | Joback Method |
| dvisc | 0.0016852 | Paxs | 236.50 | Joback Method |
| dvisc | 0.0009040 | Paxs | 272.51 | Joback Method |
| dvisc | 0.0005608 | Paxs | 308.51 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0003844 | Paxs | 344.52 | Joback Method |
| dvisc | 0.0002831 | Paxs | 380.53 | Joback Method |
| dvisc | 0.0002197 | Paxs | 416.54 | 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=C5910850&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |
| ripol: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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