

# 2,4-Undecadienal, (E,E)-

|                      |                                                                                                                                                                                                                                                          |
|----------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 2,4-trans,trans-Undecadienal<br>2,4-Undecadien-1-al<br>trans,trans-2,4-Undecadien-1-al<br>(E,E)-2,4-Undecadien-1-al<br>(2E,4E)-2,4-Undecadienal<br>(E,E)-2,4-Undecadienal<br>(E,E)-Undeca-2,4-dienal<br>(E,E)-2,4-Undecanal<br>(2E,4E)-undeca-2,4-dienal |
| Inchi:               | InChI=1S/C11H18O/c1-2-3-4-5-6-7-8-9-10-11-12/h7-11H,2-6H2,1H3/b8-7+,10-9+                                                                                                                                                                                |
| InchiKey:            | UVIUHIFPIWRILL-XBLVEGMJSA-N                                                                                                                                                                                                                              |
| Formula:             | C11H18O                                                                                                                                                                                                                                                  |
| SMILES:              | CCCCCCC=CC=CC=O                                                                                                                                                                                                                                          |
| Mol. weight [g/mol]: | 166.26                                                                                                                                                                                                                                                   |
| CAS:                 | 30361-29-6                                                                                                                                                                                                                                               |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 102.66  | kJ/mol  | Joback Method  |
| hf            | -121.51 | kJ/mol  | Joback Method  |
| hfus          | 26.94   | kJ/mol  | Joback Method  |
| hvap          | 46.72   | kJ/mol  | Joback Method  |
| log10ws       | -3.41   |         | Crippen Method |
| logp          | 3.268   |         | Crippen Method |
| mcvol         | 158.820 | ml/mol  | McGowan Method |
| pc            | 2276.24 | kPa     | Joback Method  |
| rinpol        | 1445.00 |         | NIST Webbook   |
| rinpol        | 1416.00 |         | NIST Webbook   |
| rinpol        | 1430.00 |         | NIST Webbook   |
| rinpol        | 1445.00 |         | NIST Webbook   |
| ripol         | 1958.00 |         | NIST Webbook   |
| ripol         | 1958.00 |         | NIST Webbook   |
| ripol         | 1931.00 |         | NIST Webbook   |
| tb            | 508.06  | K       | Joback Method  |
| tc            | 690.37  | K       | Joback Method  |
| tf            | 245.57  | K       | Joback Method  |
| vc            | 0.628   | m3/kmol | Joback Method  |

# Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 354.24    | J/mol×K | 508.06          | Joback Method |
| cpg           | 368.47    | J/mol×K | 538.45          | Joback Method |
| cpg           | 381.98    | J/mol×K | 568.83          | Joback Method |
| cpg           | 394.80    | J/mol×K | 599.22          | Joback Method |
| cpg           | 406.97    | J/mol×K | 629.60          | Joback Method |
| cpg           | 418.52    | J/mol×K | 659.99          | Joback Method |
| cpg           | 429.49    | J/mol×K | 690.37          | Joback Method |
| dvisc         | 0.0044691 | Pa×s    | 245.57          | Joback Method |
| dvisc         | 0.0017841 | Pa×s    | 289.32          | Joback Method |
| dvisc         | 0.0009065 | Pa×s    | 333.07          | Joback Method |
| dvisc         | 0.0005390 | Pa×s    | 376.81          | Joback Method |
| dvisc         | 0.0003571 | Pa×s    | 420.56          | Joback Method |
| dvisc         | 0.0002557 | Pa×s    | 464.31          | Joback Method |
| dvisc         | 0.0001939 | Pa×s    | 508.06          | Joback Method |

## Sources

|                 |                                                                                                                                               |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C30361296&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C30361296&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                         |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |

## Legend

|               |                                                 |
|---------------|-------------------------------------------------|
| <b>cpg:</b>   | Ideal gas heat capacity                         |
| <b>dvisc:</b> | Dynamic viscosity                               |
| <b>gf:</b>    | Standard Gibbs free energy of formation         |
| <b>hf:</b>    | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>  | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>  | Enthalpy of vaporization at standard conditions |

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>mcvol:</b>   | McGowan's characteristic volume     |
| <b>pc:</b>      | Critical Pressure                   |
| <b>rinpol:</b>  | Non-polar retention indices         |
| <b>ripol:</b>   | Polar retention indices             |
| <b>tb:</b>      | Normal Boiling Point Temperature    |
| <b>tc:</b>      | Critical Temperature                |
| <b>tf:</b>      | Normal melting (fusion) point       |
| <b>vc:</b>      | Critical Volume                     |

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