

# Tricyclo[4.2.0.0<sup>2,5</sup>]oct-3-ene,(1&#945

|                      |                                                       |
|----------------------|-------------------------------------------------------|
| Other names:         | Tricyclo[4.2.0.0                                      |
| Inchi:               | InChI=1S/C8H10/c1-2-6-5(1)7-3-4-8(6)7/h1-2,5-8H,3-4H2 |
| InchiKey:            | YHCXYJYRBADQSN-UHFFFAOYSA-N                           |
| Formula:             | C8H10                                                 |
| SMILES:              | C1=CC2C1C1CCC21                                       |
| Mol. weight [g/mol]: | 106.17                                                |
| CAS:                 | 39781-76-5                                            |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 233.08  | kJ/mol  | Joback Method  |
| hf            | 53.55   | kJ/mol  | Joback Method  |
| hfus          | 15.27   | kJ/mol  | Joback Method  |
| hvap          | 32.95   | kJ/mol  | Joback Method  |
| ie            | 9.25    | eV      | NIST Webbook   |
| log10ws       | -1.74   |         | Crippen Method |
| logp          | 1.828   |         | Crippen Method |
| mcvol         | 86.700  | ml/mol  | McGowan Method |
| pc            | 3819.82 | kPa     | Joback Method  |
| tb            | 392.88  | K       | Joback Method  |
| tc            | 596.21  | K       | Joback Method  |
| tf            | 233.78  | K       | Joback Method  |
| vc            | 0.347   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 174.43 | J/mol×K | 392.88          | Joback Method |
| cpg           | 190.64 | J/mol×K | 426.77          | Joback Method |
| cpg           | 205.57 | J/mol×K | 460.66          | Joback Method |
| cpg           | 219.33 | J/mol×K | 494.55          | Joback Method |
| cpg           | 231.99 | J/mol×K | 528.44          | Joback Method |
| cpg           | 243.65 | J/mol×K | 562.32          | Joback Method |
| cpg           | 254.40 | J/mol×K | 596.21          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001254 | Pa×s | 233.78 | Joback Method |
| dvisc | 0.0001973 | Pa×s | 260.30 | Joback Method |
| dvisc | 0.0002855 | Pa×s | 286.81 | Joback Method |
| dvisc | 0.0003881 | Pa×s | 313.33 | Joback Method |
| dvisc | 0.0005030 | Pa×s | 339.85 | Joback Method |
| dvisc | 0.0006277 | Pa×s | 366.36 | Joback Method |
| dvisc | 0.0007604 | Pa×s | 392.88 | Joback Method |

## Sources

|                        |                                                                                                                                               |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                         |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C39781765&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C39781765&amp;Units=SI</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>ie:</b>      | Ionization energy                               |
| <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>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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