

# Tricyclo[4.2.2.0<sup>2,5</sup>]decane,7,8-bis(m

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Tricyclo[4.2.2.0   |
| <b>Inchi:</b>               | InChI=1S/C12H16/c1-7-8(2)12-10-5-3-9(4-6-10)11(7)12/h9-12H,1-6H2 |
| <b>InchiKey:</b>            | YUKWZNIRAABSA-UHFFFAOYSA-N                                       |
| <b>Formula:</b>             | C12H16   |
| <b>SMILES:</b>              | C=C1C(=C)C2C3CCC(CC3)C12   |
| <b>Mol. weight [g/mol]:</b> | 160.26   |
| <b>CAS:</b>                 | 36439-92-6   |

## Physical Properties

| Property code | Value       | Unit                 | Source         |
|---------------|-------------|----------------------|----------------|
| gf            | 318.76      | kJ/mol               | Joback Method  |
| hf            | 69.37       | kJ/mol               | Joback Method  |
| hfus          | 17.89       | kJ/mol               | Joback Method  |
| hvap          | 42.23       | kJ/mol               | Joback Method  |
| ie            | 8.27 ± 0.03 | eV                   | NIST Webbook   |
| log10ws       | -3.27       |                      | Crippen Method |
| logp          | 3.165       |                      | Crippen Method |
| mcvol         | 138.760     | ml/mol               | McGowan Method |
| pc            | 2629.85     | kPa                  | Joback Method  |
| tb            | 492.10      | K                    | Joback Method  |
| tc            | 703.50      | K                    | Joback Method  |
| tf            | 298.42      | K                    | Joback Method  |
| vc            | 0.537       | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 333.31 | J/mol×K | 492.10          | Joback Method |
| cpg           | 352.59 | J/mol×K | 527.33          | Joback Method |
| cpg           | 370.61 | J/mol×K | 562.57          | Joback Method |
| cpg           | 387.45 | J/mol×K | 597.80          | Joback Method |
| cpg           | 403.19 | J/mol×K | 633.04          | Joback Method |
| cpg           | 417.92 | J/mol×K | 668.27          | Joback Method |
| cpg           | 431.72 | J/mol×K | 703.50          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0008564 | Paxs | 298.42 | Joback Method |
| dvisc | 0.0009910 | Paxs | 330.70 | Joback Method |
| dvisc | 0.0011173 | Paxs | 362.98 | Joback Method |
| dvisc | 0.0012354 | Paxs | 395.26 | Joback Method |
| dvisc | 0.0013453 | Paxs | 427.54 | Joback Method |
| dvisc | 0.0014476 | Paxs | 459.82 | Joback Method |
| dvisc | 0.0015428 | Paxs | 492.10 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=C36439926&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C36439926&amp;Units=SI</a> |
| <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>   |

## 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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