

# Tricyclo[8.4.0.0(2,7)]dodecane, isomer # 4

|                      |                                                                          |
|----------------------|--------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C14H24/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)13/h11-14H,1-10H2 |
| InchiKey:            | GNMCGMFNBARSY-UHFFFAOYSA-N                                               |
| Formula:             | C14H24                                                                   |
| SMILES:              | C1CCC2C(C1)CCC1CCCCC12                                                   |
| Mol. weight [g/mol]: | 192.34                                                                   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 181.04  | kJ/mol  | Joback Method  |
| hf            | -165.03 | kJ/mol  | Joback Method  |
| hfus          | 16.99   | kJ/mol  | Joback Method  |
| hvap          | 47.05   | kJ/mol  | Joback Method  |
| log10ws       | -4.40   |         | Crippen Method |
| logp          | 4.393   |         | Crippen Method |
| mcvol         | 175.540 | ml/mol  | McGowan Method |
| pc            | 2311.39 | kPa     | Joback Method  |
| rinpol        | 1552.00 |         | NIST Webbook   |
| rinpol        | 1575.00 |         | NIST Webbook   |
| rinpol        | 1552.00 |         | NIST Webbook   |
| tb            | 556.62  | K       | Joback Method  |
| tc            | 789.03  | K       | Joback Method  |
| tf            | 279.52  | K       | Joback Method  |
| vc            | 0.649   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 476.02 | J/mol×K | 556.62          | Joback Method |
| cpg           | 503.38 | J/mol×K | 595.35          | Joback Method |
| cpg           | 528.90 | J/mol×K | 634.09          | Joback Method |
| cpg           | 552.65 | J/mol×K | 672.82          | Joback Method |
| cpg           | 574.73 | J/mol×K | 711.56          | Joback Method |
| cpg           | 595.25 | J/mol×K | 750.29          | Joback Method |
| cpg           | 614.30 | J/mol×K | 789.03          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0033535 | Pa×s | 279.52 | Joback Method |
| dvisc | 0.0021240 | Pa×s | 325.70 | Joback Method |
| dvisc | 0.0015068 | Pa×s | 371.89 | Joback Method |
| dvisc | 0.0011532 | Pa×s | 418.07 | Joback Method |
| dvisc | 0.0009308 | Pa×s | 464.25 | Joback Method |
| dvisc | 0.0007810 | Pa×s | 510.44 | Joback Method |
| dvisc | 0.0006747 | Pa×s | 556.62 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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=R524691&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R524691&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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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