

# 4,4,7,7-Tetramethylcyclodecene trans

|                      |                                                                                 |
|----------------------|---------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C14H26/c1-13(2)9-7-5-6-8-10-14(3,4)12-11-13/h5,7H,6,8-12H2,1-4H3/b7-5+ |
| InchiKey:            | XUWUSDXUASTJCZ-FNORWQNLSA-N                                                     |
| Formula:             | C14H26                                                                          |
| SMILES:              | CC1(C)CC=CCCC(C)(C)CC1                                                          |
| Mol. weight [g/mol]: | 194.36                                                                          |
| CAS:                 | 2198-43-8                                                                       |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 54.32   | kJ/mol  | Joback Method  |
| hf            | -234.69 | kJ/mol  | Joback Method  |
| hfus          | 5.15    | kJ/mol  | Joback Method  |
| hvap          | 45.56   | kJ/mol  | Joback Method  |
| log10ws       | -4.95   |         | Crippen Method |
| logp          | 4.949   |         | Crippen Method |
| mcvol         | 192.960 | ml/mol  | McGowan Method |
| pc            | 2135.43 | kPa     | Joback Method  |
| tb            | 551.32  | K       | Joback Method  |
| tc            | 787.24  | K       | Joback Method  |
| tf            | 285.16  | K       | Joback Method  |
| vc            | 0.702   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 483.66 | J/mol×K | 551.32          | Joback Method |
| cpg           | 509.66 | J/mol×K | 590.64          | Joback Method |
| cpg           | 534.00 | J/mol×K | 629.96          | Joback Method |
| cpg           | 556.91 | J/mol×K | 669.28          | Joback Method |
| cpg           | 578.61 | J/mol×K | 708.60          | Joback Method |
| cpg           | 599.33 | J/mol×K | 747.92          | Joback Method |
| cpg           | 619.29 | J/mol×K | 787.24          | 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=C2198438&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2198438&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>                                   |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <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>hvac:</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>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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