

# 1-[(5E)-1,4,7,10,14,15-hexamethyl-11-methylene-4-

InChI: Isomer # 1 InChI=1S/C34H58/c1-13-34(12,23-21-30(8)32-19-18-31(9)33(10,11)24-32)22-20-26(4)14  
InChIKey: IBJRNORNAWSUOG-LSDHQDQOSA-N

Formula: C34H58  
SMILES: C=CC(C)(C=CC(C)CCC(C)C(=C)CCC(C)C(=C)C)CCC(C)C1=CC(C)(C)C(C)CC1  
Mol. weight [g/mol]: 466.82

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 586.70  | kJ/mol  | Joback Method  |
| hf            | -205.50 | kJ/mol  | Joback Method  |
| hfus          | 43.49   | kJ/mol  | Joback Method  |
| hvap          | 86.46   | kJ/mol  | Joback Method  |
| log10ws       | -11.53  |         | Crippen Method |
| logp          | 11.135  |         | Crippen Method |
| mcvol         | 457.560 | ml/mol  | McGowan Method |
| pc            | 623.44  | kPa     | Joback Method  |
| rinpol        | 2745.00 |         | NIST Webbook   |
| rinpol        | 2748.00 |         | NIST Webbook   |
| tb            | 985.55  | K       | Joback Method  |
| tc            | 1206.92 | K       | Joback Method  |
| tf            | 417.40  | K       | Joback Method  |
| vc            | 1.746   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1613.52 | J/mol×K | 985.55          | Joback Method |
| cpg           | 1642.96 | J/mol×K | 1022.45         | Joback Method |
| cpg           | 1672.09 | J/mol×K | 1059.34         | Joback Method |
| cpg           | 1701.15 | J/mol×K | 1096.24         | Joback Method |
| cpg           | 1730.39 | J/mol×K | 1133.13         | Joback Method |
| cpg           | 1760.07 | J/mol×K | 1170.03         | Joback Method |
| cpg           | 1790.43 | J/mol×K | 1206.92         | 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=R586377&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R586377&amp;Units=SI</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>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>rlnpol:</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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