

# cis-7,8-epoxy-2-methyl-Z12-octadecene

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C19H36O/c1-4-5-6-7-8-9-10-11-15-18-19(20-18)16-13-12-14-17(2)3/h8-9,17-1 |
| <b>InchiKey:</b>            | MRJWGCAZSVVLNB-HJWRWDBZSA-N   |
| <b>Formula:</b>             | C19H36O   |
| <b>SMILES:</b>              | CCCCC=CCCC1OC1CCCC(C)C  |
| <b>Mol. weight [g/mol]:</b> | 280.49  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 153.80  | kJ/mol  | Joback Method  |
| hf            | -403.09 | kJ/mol  | Joback Method  |
| hfus          | 48.83   | kJ/mol  | Joback Method  |
| hvap          | 61.57   | kJ/mol  | Joback Method  |
| log10ws       | -6.59   |         | Crippen Method |
| logp          | 6.277   |         | Crippen Method |
| mcvol         | 269.280 | ml/mol  | McGowan Method |
| pc            | 1194.00 | kPa     | Joback Method  |
| rinpol        | 2005.00 |         | NIST Webbook   |
| tb            | 666.86  | K       | Joback Method  |
| tc            | 841.46  | K       | Joback Method  |
| tf            | 324.08  | K       | Joback Method  |
| vc            | 1.050   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 788.54    | J/molxK | 666.86          | Joback Method |
| cpg           | 809.13    | J/molxK | 695.96          | Joback Method |
| cpg           | 828.75    | J/molxK | 725.06          | Joback Method |
| cpg           | 847.45    | J/molxK | 754.16          | Joback Method |
| cpg           | 865.28    | J/molxK | 783.26          | Joback Method |
| cpg           | 882.29    | J/molxK | 812.36          | Joback Method |
| cpg           | 898.52    | J/molxK | 841.46          | Joback Method |
| dvisc         | 0.0030466 | Paxs    | 324.08          | Joback Method |
| dvisc         | 0.0014694 | Paxs    | 381.21          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0008570 | Paxs | 438.34 | Joback Method |
| dvisc | 0.0005660 | Paxs | 495.47 | Joback Method |
| dvisc | 0.0004073 | Paxs | 552.60 | Joback Method |
| dvisc | 0.0003118 | Paxs | 609.73 | Joback Method |
| dvisc | 0.0002498 | Paxs | 666.86 | 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=R413739&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R413739&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>                                 |
| <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>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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