

(E,  
E)-3,7,11-Trimethyl-7,10-epoxydodeca-2,5,11-trien  
acetate

Inchi: InChI=1S/C17H26O3/c1-13(2)16-8-11-17(5,20-16)10-6-7-14(3)9-12-19-15(4)18/h6,9-10,  
InchiKey: UJWIEJULEWRZEG-WNUTZXNYS-A-N  
Formula: C17H26O3  
SMILES: C=C(C)C1CCC(C)(C=CCC(C)=CCOC(C)=O)O1  
Mol. weight [g/mol]: 278.39

Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 26.75   | kJ/mol  | Joback Method  |
| hf            | -375.34 | kJ/mol  | Joback Method  |
| hfus          | 35.76   | kJ/mol  | Joback Method  |
| hvap          | 65.31   | kJ/mol  | Joback Method  |
| log10ws       | -4.57   |         | Crippen Method |
| logp          | 3.956   |         | Crippen Method |
| mcvol         | 239.940 | ml/mol  | McGowan Method |
| pc            | 1645.76 | kPa     | Joback Method  |
| rinpol        | 1816.00 |         | NIST Webbook   |
| tb            | 707.21  | K       | Joback Method  |
| tc            | 917.20  | K       | Joback Method  |
| tf            | 370.80  | K       | Joback Method  |
| vc            | 0.913   | m3/kmol | Joback Method  |

Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 688.97 | J/mol×K | 707.21          | Joback Method |
| cpg           | 707.92 | J/mol×K | 742.21          | Joback Method |
| cpg           | 726.02 | J/mol×K | 777.21          | Joback Method |
| cpg           | 743.41 | J/mol×K | 812.21          | Joback Method |
| cpg           | 760.23 | J/mol×K | 847.20          | Joback Method |
| cpg           | 776.62 | J/mol×K | 882.20          | Joback Method |
| cpg           | 792.73 | J/mol×K | 917.20          | 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=R227375&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R227375&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>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>rinpola:</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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