

# Allyl ionone 4

Inchi:

InChI=1S/C16H24O/c1-5-6-9-14(17)10-11-15-13(2)8-7-12-16(15,3)4/h5,8,10-11,15H,1,6H,2H

InchiKey:

FXCYGAGBPZQRJE-ZHACJKMWSA-N

Formula:

C16H24O

SMILES:

C=CCCC(=O)C=CC1C(C)=CCCC1(C)C

Mol. weight [g/mol]:

232.36

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 154.56  | kJ/mol  | Joback Method  |
| hf            | -147.97 | kJ/mol  | Joback Method  |
| hfus          | 25.16   | kJ/mol  | Joback Method  |
| hvap          | 57.17   | kJ/mol  | Joback Method  |
| log10ws       | -4.77   |         | Crippen Method |
| logp          | 4.460   |         | Crippen Method |
| mcvol         | 214.110 | ml/mol  | McGowan Method |
| pc            | 1796.98 | kPa     | Joback Method  |
| rinpol        | 1734.00 |         | NIST Webbook   |
| rinpol        | 1734.00 |         | NIST Webbook   |
| ripol         | 2199.00 |         | NIST Webbook   |
| ripol         | 2199.00 |         | NIST Webbook   |
| tb            | 639.45  | K       | Joback Method  |
| tc            | 850.87  | K       | Joback Method  |
| tf            | 353.49  | K       | Joback Method  |
| vc            | 0.815   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 572.70 | J/mol×K | 639.45          | Joback Method |
| cpg           | 592.10 | J/mol×K | 674.69          | Joback Method |
| cpg           | 610.47 | J/mol×K | 709.92          | Joback Method |
| cpg           | 627.94 | J/mol×K | 745.16          | Joback Method |
| cpg           | 644.64 | J/mol×K | 780.40          | Joback Method |
| cpg           | 660.70 | J/mol×K | 815.63          | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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=U284930&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U284930&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>                         |

## 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>rinpol:</b>  | Non-polar retention indices                     |
| <b>ripol:</b>   | 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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