

# «beta»-Isocyclolavandulyl isovalerate

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H26O2/c1-11(2)8-14(16)17-10-13-6-7-15(4,5)9-12(13)3/h6,11-12H,7-10H2

JRORWOF CFY WYNY-LBPRGKRZSA-N

C15H26O2

CC(C)CC(=O)OCC1=CCC(C)(C)CC1C

238.37

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -129.36 | kJ/mol  | Joback Method  |
| hf            | -507.48 | kJ/mol  | Joback Method  |
| hfus          | 21.31   | kJ/mol  | Joback Method  |
| hvap          | 57.67   | kJ/mol  | Joback Method  |
| log10ws       | -3.99   |         | Crippen Method |
| logp          | 3.958   |         | Crippen Method |
| mcvol         | 214.490 | ml/mol  | McGowan Method |
| pc            | 1786.37 | kPa     | Joback Method  |
| rinpol        | 1520.00 |         | NIST Webbook   |
| ripol         | 1788.00 |         | NIST Webbook   |
| tb            | 637.71  | K       | Joback Method  |
| tc            | 842.17  | K       | Joback Method  |
| tf            | 356.29  | K       | Joback Method  |
| vc            | 0.809   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 591.64 | J/mol×K | 637.71          | Joback Method |
| cpg           | 611.49 | J/mol×K | 671.79          | Joback Method |
| cpg           | 630.38 | J/mol×K | 705.86          | Joback Method |
| cpg           | 648.39 | J/mol×K | 739.94          | Joback Method |
| cpg           | 665.60 | J/mol×K | 774.02          | Joback Method |
| cpg           | 682.11 | J/mol×K | 808.09          | Joback Method |
| cpg           | 698.00 | J/mol×K | 842.17          | 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=R418883&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R418883&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>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>ripola:</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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