

# 3,4-Di-O-acetyl-1,5-Anhydro-2-O-methyl-L-rhamnitol

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C11H18O6/c1-6-10(16-7(2)12)11(17-8(3)13)9(14-4)5-15-6/h6,9-11H,5H2,1-4H

UURZDJOBKDXBB-JGBZZBSPSA-N

C11H18O6

COC1COC(C)C(OC(C)=O)C1OC(C)=O

246.26

## Physical Properties

| Property code | Value    | Unit    | Source         |
|---------------|----------|---------|----------------|
| gf            | -615.90  | kJ/mol  | Joback Method  |
| hf            | -1030.89 | kJ/mol  | Joback Method  |
| hfus          | 34.03    | kJ/mol  | Joback Method  |
| hvap          | 64.81    | kJ/mol  | Joback Method  |
| log10ws       | -0.67    |         | Crippen Method |
| logp          | 0.283    |         | Crippen Method |
| mcvol         | 181.610  | ml/mol  | McGowan Method |
| pc            | 2263.26  | kPa     | Joback Method  |
| rinpol        | 1492.71  |         | NIST Webbook   |
| tb            | 658.57   | K       | Joback Method  |
| tc            | 862.68   | K       | Joback Method  |
| tf            | 401.51   | K       | Joback Method  |
| vc            | 0.668    | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 521.31    | J/mol×K | 658.57          | Joback Method |
| cpg           | 538.33    | J/mol×K | 692.59          | Joback Method |
| cpg           | 554.40    | J/mol×K | 726.61          | Joback Method |
| cpg           | 569.49    | J/mol×K | 760.63          | Joback Method |
| cpg           | 583.56    | J/mol×K | 794.64          | Joback Method |
| cpg           | 596.58    | J/mol×K | 828.66          | Joback Method |
| cpg           | 608.52    | J/mol×K | 862.68          | Joback Method |
| dvisc         | 0.0012794 | Pa×s    | 401.51          | Joback Method |
| dvisc         | 0.0008278 | Pa×s    | 444.35          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0005783 | Pa×s | 487.20 | Joback Method |
| dvisc | 0.0004281 | Pa×s | 530.04 | Joback Method |
| dvisc | 0.0003314 | Pa×s | 572.88 | Joback Method |
| dvisc | 0.0002659 | Pa×s | 615.73 | Joback Method |
| dvisc | 0.0002196 | Pa×s | 658.57 | 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=R182955&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R182955&amp;Units=SI</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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