

# 3,4-dihydro-3-oxoactinidol II

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C13H20O3/c1-8(14)10-5-11-12(2,3)6-9(15)7-13(11,4)16-10/h5,8,10,14H,6-7H2

GQMVJMPTJNNDRV-RHYVWVDMSA-N

C13H20O3

CC(O)C1C=C2C(C)(C)CC(=O)CC2(C)O1

224.30

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -202.55 | kJ/mol  | Joback Method  |
| hf            | -555.29 | kJ/mol  | Joback Method  |
| hfus          | 16.76   | kJ/mol  | Joback Method  |
| hvap          | 68.26   | kJ/mol  | Joback Method  |
| log10ws       | -2.63   |         | Crippen Method |
| logp          | 1.840   |         | Crippen Method |
| mcvol         | 181.320 | ml/mol  | McGowan Method |
| pc            | 2693.00 | kPa     | Joback Method  |
| ripol         | 2456.00 |         | NIST Webbook   |
| ripol         | 2456.00 |         | NIST Webbook   |
| tb            | 709.59  | K       | Joback Method  |
| tc            | 931.33  | K       | Joback Method  |
| tf            | 459.04  | K       | Joback Method  |
| vc            | 0.675   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 548.07 | J/molxK | 709.59          | Joback Method |
| cpg           | 564.84 | J/molxK | 746.55          | Joback Method |
| cpg           | 581.20 | J/molxK | 783.50          | Joback Method |
| cpg           | 597.35 | J/molxK | 820.46          | Joback Method |
| cpg           | 613.50 | J/molxK | 857.42          | Joback Method |
| cpg           | 629.87 | J/molxK | 894.37          | Joback Method |
| cpg           | 646.65 | J/molxK | 931.33          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R332888&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R332888&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>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>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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