

# 2-Naphthalenol, acetate

|                      |                                                                                                                                                                                                                                                               |
|----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 2-Naphthol, acetate<br>«beta»-Naphthol acetate<br>«beta»-Naphthyl acetate<br>Naphthalene, 2-acetoxy-<br>O-Acetyl-«beta»-naphthol<br>2-Acetoxynaphthalene<br>2-Naphthyl acetate<br>Acetic acid «beta»-naphthyl ester<br>2-Naphthalenol, 2-acetate<br>NSC 37069 |
| Inchi:               | InChI=1S/C12H10O2/c1-9(13)14-12-7-6-10-4-2-3-5-11(10)8-12/h2-8H,1H3                                                                                                                                                                                           |
| InchiKey:            | RJNPPEUAJCEUPV-UHFFFAOYSA-N                                                                                                                                                                                                                                   |
| Formula:             | C12H10O2                                                                                                                                                                                                                                                      |
| SMILES:              | CC(=O)Oc1ccc2ccccc2c1                                                                                                                                                                                                                                         |
| Mol. weight [g/mol]: | 186.21                                                                                                                                                                                                                                                        |
| CAS:                 | 1523-11-1                                                                                                                                                                                                                                                     |

## Physical Properties

| Property code | Value           | Unit   | Source         |
|---------------|-----------------|--------|----------------|
| chs           | -5847.00 ± 2.40 | kJ/mol | NIST Webbook   |
| chs           | -5841.70 ± 1.10 | kJ/mol | NIST Webbook   |
| gf            | 25.67           | kJ/mol | Joback Method  |
| hf            | -119.68         | kJ/mol | Joback Method  |
| hfs           | -309.60 ± 1.10  | kJ/mol | NIST Webbook   |
| hfus          | 20.29           | kJ/mol | Joback Method  |
| hsub          | 96.30 ± 0.60    | kJ/mol | NIST Webbook   |
| hvap          | 56.04           | kJ/mol | Joback Method  |
| log10ws       | -3.59           |        | Crippen Method |
| logp          | 2.765           |        | Crippen Method |
| mcvol         | 144.160         | ml/mol | McGowan Method |
| pc            | 3217.33         | kPa    | Joback Method  |
| rinpol        | 1585.00         |        | NIST Webbook   |
| rinpol        | 1585.00         |        | NIST Webbook   |
| rinpol        | 1585.00         |        | NIST Webbook   |
| tb            | 600.89          | K      | Joback Method  |
| tc            | 836.14          | K      | Joback Method  |
| tf            | 342.00 ± 0.50   | K      | NIST Webbook   |

|    |       |                      |               |
|----|-------|----------------------|---------------|
| vc | 0.545 | m <sup>3</sup> /kmol | Joback Method |
|----|-------|----------------------|---------------|

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 393.88    | J/mol×K | 796.93          | Joback Method |
| cpg           | 402.88    | J/mol×K | 836.14          | Joback Method |
| cpg           | 336.63    | J/mol×K | 600.89          | Joback Method |
| cpg           | 349.90    | J/mol×K | 640.10          | Joback Method |
| cpg           | 362.21    | J/mol×K | 679.31          | Joback Method |
| cpg           | 373.60    | J/mol×K | 718.51          | Joback Method |
| cpg           | 384.14    | J/mol×K | 757.72          | Joback Method |
| dvisc         | 0.0002966 | Pa×s    | 600.89          | Joback Method |
| dvisc         | 0.0003519 | Pa×s    | 562.21          | Joback Method |
| dvisc         | 0.0014170 | Pa×s    | 368.80          | Joback Method |
| dvisc         | 0.0009648 | Pa×s    | 407.48          | Joback Method |
| dvisc         | 0.0007022 | Pa×s    | 446.16          | Joback Method |
| dvisc         | 0.0005377 | Pa×s    | 484.85          | Joback Method |
| dvisc         | 0.0004282 | Pa×s    | 523.53          | Joback Method |
| hfust         | 20.05     | kJ/mol  | 342.20          | NIST Webbook  |
| hfust         | 20.05     | kJ/mol  | 342.20          | NIST Webbook  |

## Sources

|                 |                                                                                                                                             |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                   |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                       |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1523111&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1523111&amp;Units=SI</a> |

## Legend

|        |                                         |
|--------|-----------------------------------------|
| chs:   | Standard solid enthalpy of combustion   |
| cpg:   | Ideal gas heat capacity                 |
| dvisc: | Dynamic viscosity                       |
| gf:    | Standard Gibbs free energy of formation |

|                 |                                                          |
|-----------------|----------------------------------------------------------|
| <b>hf:</b>      | Enthalpy of formation at standard conditions             |
| <b>hfs:</b>     | Solid phase enthalpy of formation at standard conditions |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions                |
| <b>hfust:</b>   | Enthalpy of fusion at a given temperature                |
| <b>hsub:</b>    | Enthalpy of sublimation 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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