

# 1-Acetamido-2-methyl-naphthalene

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C13H13NO/c1-9-7-8-11-5-3-4-6-12(11)13(9)14-10(2)15/h3-8H,1-2H3,(H,14,15) |
| InchiKey:            | SGRWRTKJEQTSCK-UHFFFAOYSA-N                                                       |
| Formula:             | C13H13NO                                                                          |
| SMILES:              | CC(O)=Nc1c(C)ccc2ccccc12                                                          |
| Mol. weight [g/mol]: | 199.25                                                                            |
| CAS:                 | 13615-35-5                                                                        |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | 13.21   | kJ/mol | Joback Method  |
| hvap          | 69.85   | kJ/mol | Joback Method  |
| log10ws       | -4.14   |        | Crippen Method |
| logp          | 3.756   |        | Crippen Method |
| mcvol         | 162.360 | ml/mol | McGowan Method |
| pc            | 2690.21 | kPa    | Joback Method  |
| tb            | 721.20  | K      | Joback Method  |
| tc            | 947.92  | K      | Joback Method  |

## Sources

|                 |                                                                                                                                               |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| 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=C13615355&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13615355&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                     |

## Legend

|          |                                                 |
|----------|-------------------------------------------------|
| hf:      | Enthalpy of formation at standard conditions    |
| hvap:    | Enthalpy of vaporization at standard conditions |
| log10ws: | 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>tb:</b>    | Normal Boiling Point Temperature    |
| <b>tc:</b>    | Critical Temperature                |

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