

# Acetamide, N-(2,5-dimethylphenyl)-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Acetanilide, 2',5'-dimethyl-<br>2,5-Dimethylacetanilide<br>2',5'-Acetoxyidide<br>2',5'-Dimethylacetanilide<br>2,5-DMA<br>N-(2,5-Dimethylphenyl)acetamide |
| <b>Inchi:</b>               | InChI=1S/C10H13NO/c1-7-4-5-8(2)10(6-7)11-9(3)12/h4-6H,1-3H3,(H,11,12)  |
| <b>InchiKey:</b>            | CXLKSNKWHULUKA-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C10H13NO   |
| <b>SMILES:</b>              | <chem>CC(O)=Nc1cc(C)ccc1C</chem>   |
| <b>Mol. weight [g/mol]:</b> | 163.22   |
| <b>CAS:</b>                 | 2050-44-4  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | -115.94 | kJ/mol | Joback Method  |
| hvap          | 61.53   | kJ/mol | Joback Method  |
| log10ws       | -2.81   |        | Crippen Method |
| logp          | 2.911   |        | Crippen Method |
| mcvol         | 139.550 | ml/mol | McGowan Method |
| pc            | 2814.34 | kPa    | Joback Method  |
| rinpola       | 1591.00 |        | NIST Webbook   |
| rinpola       | 1591.00 |        | NIST Webbook   |
| tb            | 633.58  | K      | Joback Method  |
| tc            | 846.49  | K      | Joback Method  |

## Sources

|                        |   |
|------------------------|---|
| <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=C2050444&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2050444&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>                                       |

# Legend

|                            |   |
|----------------------------|---|
| <b>hf:</b>                 | Enthalpy of formation at standard conditions    |
| <b>h<sub>vap</sub>:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log<sub>10</sub>ws:</b> | Log <sub>10</sub> of Water solubility in mol/l  |
| <b>log<sub>p</sub>:</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                            |

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