

# Diacetamate

|                      |                                                                                                                                                                                                                                                                                                                                                                                                   |
|----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Acetamide, N-[4-(acetyloxy)phenyl]-<br>p-Acetoxyacetanilide<br>Acetaminophen acetate<br>Acetanilide, 4'-hydroxy-, acetate (ester)<br>Diacetamat<br>N-Acetyl-4-aminophenyl acetate<br>4-Acetamidophenyl acetate<br>4-Acetoxyacetanilide<br>4-(Acetylamino)phenyl acetate<br>Acetanilide, 4'-hydroxy-, acetate<br>NSC 33893<br>NSC 6083<br>O-Acetylparacetamol<br>N-[4-(acetyloxy)phenyl] acetamide |
| Inchi:               | InChI=1S/C10H11NO3/c1-7(12)11-9-3-5-10(6-4-9)14-8(2)13/h3-6H,1-2H3,(H,11,12)                                                                                                                                                                                                                                                                                                                      |
| InchiKey:            | UJAOSPFULOFZRR-UHFFFAOYSA-N                                                                                                                                                                                                                                                                                                                                                                       |
| Formula:             | C10H11NO3                                                                                                                                                                                                                                                                                                                                                                                         |
| SMILES:              | CC(=O)Oc1ccc(N=C(C)O)cc1                                                                                                                                                                                                                                                                                                                                                                          |
| Mol. weight [g/mol]: | 193.20                                                                                                                                                                                                                                                                                                                                                                                            |
| CAS:                 | 2623-33-8                                                                                                                                                                                                                                                                                                                                                                                         |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | -349.27 | kJ/mol | Joback Method  |
| hvap          | 70.02   | kJ/mol | Joback Method  |
| log10ws       | -2.17   |        | Crippen Method |
| logp          | 2.220   |        | Crippen Method |
| mcvol         | 146.990 | ml/mol | McGowan Method |
| pc            | 3005.73 | kPa    | Joback Method  |
| rinpol        | 1765.00 |        | NIST Webbook   |
| rinpol        | 1765.00 |        | NIST Webbook   |
| tb            | 704.89  | K      | Joback Method  |
| tc            | 920.98  | K      | Joback Method  |

# Temperature Dependent Properties

| Property code | Value | Unit   | Temperature [K] | Source       |
|---------------|-------|--------|-----------------|--------------|
| hfust         | 30.97 | kJ/mol | 427.50          | NIST Webbook |

## Sources

|                 |                                                                                                                                             |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2623338&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2623338&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>                       |

## Legend

|          |                                                 |
|----------|-------------------------------------------------|
| hf:      | Enthalpy of formation at standard conditions    |
| hfust:   | Enthalpy of fusion at a given temperature       |
| hvap:    | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l              |
| logp:    | Octanol/Water partition coefficient             |
| mcvol:   | McGowan's characteristic volume                 |
| pc:      | Critical Pressure                               |
| rinpol:  | Non-polar retention indices                     |
| tb:      | Normal Boiling Point Temperature                |
| tc:      | Critical Temperature                            |

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