

# Acetamide, 2-(diethylamino)-N-(2,4,6-trimethylphenyl)-

|                      |                                                                                                                                                                                                                                                                                                                                                                                     |
|----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Acetamide, 2-(diethylamino)-N-(2,4,6-trimethylphenyl)-<br>Acetanilide, 2-(diethylamino)-2',4',6'-trimethyl-<br>«omega»-Diethylaminoacetylaminomesitylene<br>Diethylglycinemesidide<br>Justecaina<br>Mesdicain<br>Mesidicaine<br>Mesokain<br>N-(Diethylaminoacetyl)-2,4,6-trimethylaniline<br>Trimecain<br>Trimekain<br>2-(Diethylamino)-2',4',6'-trimethylacetanilide<br>Mesidicain |
| Inchi:               | InChI=1S/C15H24N2O/c1-6-17(7-2)10-14(18)16-15-12(4)8-11(3)9-13(15)5/h8-9H,6-7,10                                                                                                                                                                                                                                                                                                    |
| InchiKey:            | GOZBHBFUQHMKQB-UHFFFAOYSA-N                                                                                                                                                                                                                                                                                                                                                         |
| Formula:             | C15H24N2O                                                                                                                                                                                                                                                                                                                                                                           |
| SMILES:              | CCN(CC)CC(=O)Nc1c(C)cc(C)cc1C                                                                                                                                                                                                                                                                                                                                                       |
| Mol. weight [g/mol]: | 248.37                                                                                                                                                                                                                                                                                                                                                                              |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| hfus          | 37.20   | kJ/mol | Joback Method      |
| ie            | 7.24    | eV     | Cheméo Relay (1.0) |
| log10ws       | -2.54   |        | Cheméo Relay (1.0) |
| logp          | 2.892   |        | Crippen Method     |
| mcvol         | 219.980 | ml/mol | McGowan Method     |
| rinpol        | 1968.00 |        | NIST Webbook       |
| rinpol        | 1974.00 |        | NIST Webbook       |
| rinpol        | 1971.00 |        | NIST Webbook       |
| rinpol        | 1971.00 |        | NIST Webbook       |
| tf            | 361.74  | K      | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 613.67 | J/mol×K | 700.70          | Joback Method |
| cpg           | 629.97 | J/mol×K | 734.05          | Joback Method |
| cpg           | 645.33 | J/mol×K | 767.39          | Joback Method |
| cpg           | 659.80 | J/mol×K | 800.74          | Joback Method |
| cpg           | 673.40 | J/mol×K | 834.09          | Joback Method |
| cpg           | 686.18 | J/mol×K | 867.44          | Joback Method |
| cpg           | 698.17 | J/mol×K | 900.78          | Joback Method |

## Sources

|                                  |                                                                                                                                           |
|----------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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>                     |
| <b>Crippen Method:</b>           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>Cheméo Relay (1.0):</b>       |                                                                                                                                           |
| <b>Cheméo Relay (1.0, beta):</b> |                                                                                                                                           |
| <b>NIST Webbook:</b>             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C616682&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C616682&amp;Units=SI</a> |

## Legend

|                 |                                           |
|-----------------|-------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                   |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions |
| <b>ie:</b>      | Ionization energy                         |
| <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>rinpol:</b>  | Non-polar retention indices               |
| <b>tf:</b>      | Normal melting (fusion) point             |

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