

# Acetamide, n-tetrahydrofurfuryl-2-methoxy-

|                      |                                                                        |
|----------------------|------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C8H15NO3/c1-11-6-8(10)9-5-7-3-2-4-12-7/h7H,2-6H2,1H3,(H,9,10) |
| InchiKey:            | ZMLJVGQFLGGFRD-UHFFFAOYSA-N                                            |
| Formula:             | C8H15NO3                                                               |
| SMILES:              | COCC(=O)NCC1CCCO1                                                      |
| Mol. weight [g/mol]: | 173.21                                                                 |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| hf            | -528.42 | kJ/mol | Cheméo Relay (1.0) |
| hfus          | 26.28   | kJ/mol | Joback Method      |
| hvap          | 67.54   | kJ/mol | Cheméo Relay (1.0) |
| logp          | -0.072  |        | Crippen Method     |
| mcvol         | 136.010 | ml/mol | McGowan Method     |
| rinpol        | 1403.00 |        | NIST Webbook       |
| rinpol        | 1403.00 |        | NIST Webbook       |
| tb            | 539.29  | K      | Cheméo Relay (1.0) |
| tf            | 306.63  | K      | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 343.22 | J/mol×K | 551.13          | Joback Method |
| cpg           | 357.91 | J/mol×K | 585.07          | Joback Method |
| cpg           | 371.82 | J/mol×K | 619.01          | Joback Method |
| cpg           | 384.98 | J/mol×K | 652.95          | Joback Method |
| cpg           | 397.39 | J/mol×K | 686.89          | Joback Method |
| cpg           | 409.07 | J/mol×K | 720.83          | Joback Method |
| cpg           | 420.03 | J/mol×K | 754.77          | 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=U307255&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307255&amp;Units=SI</a> |

## Legend

|                |                                                 |
|----------------|-------------------------------------------------|
| <b>cpg:</b>    | Ideal gas heat capacity                         |
| <b>hf:</b>     | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>   | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>   | Enthalpy of vaporization at standard conditions |
| <b>logp:</b>   | Octanol/Water partition coefficient             |
| <b>mcvol:</b>  | McGowan's characteristic volume                 |
| <b>rinpol:</b> | Non-polar retention indices                     |
| <b>tb:</b>     | Normal Boiling Point Temperature                |
| <b>tf:</b>     | Normal melting (fusion) point                   |

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