

# Acetamide, 2-chloro-N,N-di-2-propenyl-

|                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|----------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Acetamide, N,N-diallyl-2-chloro-<br>«alpha»-Chloro-N,N-diallylacetamide<br>Alidochlor<br>CDAA<br>CP 6,343<br>N-Diallyl-2-Chloroacetamide<br>N,N-Diallyl-«alpha»-chloroacetamide<br>N,N-Diallyl-2-chloroacetamide<br>N,N-Diallylchloroacetamide<br>Radox<br>Randox<br>2-Chloro-N,N-diallylacetamide<br>Acetamide, 2-chloro-N,N-diallyl-<br>Alidochlor<br>Alidochlore<br>Cdaat<br>2-Chloro-N,N-di-2-propenylacetamide<br>Diallylamid kyseliny chloroctove<br>Diallylchloroacetamide<br>NCI-C04035<br>Rantox T<br>Acetamide, 2-chloro-N,N-di-2-propen-1-yl- |
| Inchi:               | InChI=1S/C8H12ClNO/c1-3-5-10(6-4-2)8(11)7-9/h3-4H,1-2,5-7H2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| InchiKey:            | MDBGGTQNNUOQRC-UHFFFAOYSA-N                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| Formula:             | C8H12ClNO                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| SMILES:              | C=CCN(CC=C)C(=O)CCl                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| Mol. weight [g/mol]: | 173.64                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| CAS:                 | 93-71-0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |

## Physical Properties

| Property code | Value  | Unit   | Source         |
|---------------|--------|--------|----------------|
| gf            | 162.09 | kJ/mol | Joback Method  |
| hf            | -18.38 | kJ/mol | Joback Method  |
| hfus          | 22.73  | kJ/mol | Joback Method  |
| hvap          | 45.24  | kJ/mol | Joback Method  |
| log10ws       | -1.38  |        | Crippen Method |

|       |         |         |                |
|-------|---------|---------|----------------|
| logp  | 1.426   |         | Crippen Method |
| mcvol | 138.770 | ml/mol  | McGowan Method |
| pc    | 2835.36 | kPa     | Joback Method  |
| tb    | 479.54  | K       | Joback Method  |
| tc    | 666.53  | K       | Joback Method  |
| tf    | 288.72  | K       | Joback Method  |
| vc    | 0.518   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 281.33 | J/mol×K | 479.54          | Joback Method |
| cpg           | 293.03 | J/mol×K | 510.70          | Joback Method |
| cpg           | 304.09 | J/mol×K | 541.87          | Joback Method |
| cpg           | 314.53 | J/mol×K | 573.03          | Joback Method |
| cpg           | 324.38 | J/mol×K | 604.20          | Joback Method |
| cpg           | 333.67 | J/mol×K | 635.36          | Joback Method |
| cpg           | 342.42 | J/mol×K | 666.53          | 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=C93710&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C93710&amp;Units=SI</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>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                   |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <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>log10ws:</b> | 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                |
| <b>tf:</b>    | Normal melting (fusion) point       |
| <b>vc:</b>    | Critical Volume                     |

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