

# N-Ethyl-N'-(3-dimethylaminopropyl)carbodiimide

|                      |                                                                                                                                                                   |
|----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | [3-(Dimethylamino)propyl]ethylcarbodiimide<br>N3-Ethyliminomethylene-N1,N1-dimethylpropane-1,3-diamine<br>N'-(ethylcarbonimidoyl)-N,N-dimethylpropane-1,3-diamine |
| Inchi:               | InChI=1S/C8H17N3/c1-4-9-8-10-6-5-7-11(2)3/h4-7H2,1-3H3                                                                                                            |
| InchiKey:            | LMDZBCPBFSXMTL-UHFFFAOYSA-N                                                                                                                                       |
| Formula:             | C8H17N3                                                                                                                                                           |
| SMILES:              | CCN=C=NCCCN(C)C                                                                                                                                                   |
| Mol. weight [g/mol]: | 155.25                                                                                                                                                            |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| ie            | 7.61    | eV     | Cheméo Relay (1.0) |
| logp          | 1.132   |        | Crippen Method     |
| mcvol         | 144.920 | ml/mol | McGowan Method     |
| tb            | 469.19  | K      | Cheméo Relay (1.0) |

## Sources

|                           |                                                                                                                                             |
|---------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method:           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>                           |
| Cheméo Relay (1.0):       |                                                                                                                                             |
| Cheméo Relay (1.0, beta): |                                                                                                                                             |
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1892575&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1892575&amp;Units=SI</a> |
| Joback Method:            | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                       |

## Legend

|        |                                     |
|--------|-------------------------------------|
| ie:    | Ionization energy                   |
| logp:  | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume     |

**tb:** Normal Boiling Point Temperature

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