

# di-n-Decylamine

|                      |                                                                                    |
|----------------------|------------------------------------------------------------------------------------|
| Other names:         | 1-Decanamine, N-decyl-<br>Armeen 2-10<br>Didecylamine<br>Radiamine 6310            |
| Inchi:               | InChI=1S/C20H43N/c1-3-5-7-9-11-13-15-17-19-21-20-18-16-14-12-10-8-6-4-2/h21H,3-20H |
| InchiKey:            | GMTCPFCMAHMEMT-UHFFFAOYSA-N                                                        |
| Formula:             | C20H43N                                                                            |
| SMILES:              | CCCCCCCCCNCCCCCCCCC                                                                |
| Mol. weight [g/mol]: | 297.56                                                                             |
| CAS:                 | 1120-49-6                                                                          |

## Physical Properties

| Property code | Value         | Unit    | Source         |
|---------------|---------------|---------|----------------|
| gf            | 206.91        | kJ/mol  | Joback Method  |
| hf            | -402.66       | kJ/mol  | Joback Method  |
| hfus          | 52.65         | kJ/mol  | Joback Method  |
| hvap          | 66.55         | kJ/mol  | Joback Method  |
| log10ws       | -7.38         |         | Crippen Method |
| logp          | 6.857         |         | Crippen Method |
| mcvol         | 302.640       | ml/mol  | McGowan Method |
| pc            | 1024.00       | kPa     | Joback Method  |
| rinpol        | 2142.00       |         | NIST Webbook   |
| tb            | 637.15 ± 3.00 | K       | NIST Webbook   |
| tc            | 873.43        | K       | Joback Method  |
| tf            | 315.40 ± 2.00 | K       | NIST Webbook   |
| tf            | 305.75 ± 0.50 | K       | NIST Webbook   |
| tf            | 319.65 ± 3.00 | K       | NIST Webbook   |
| tf            | 321.15 ± 5.00 | K       | NIST Webbook   |
| tf            | 305.75 ± 1.00 | K       | NIST Webbook   |
| tf            | 314.65 ± 1.00 | K       | NIST Webbook   |
| tf            | 320.65 ± 5.00 | K       | NIST Webbook   |
| vc            | 1.190         | m3/kmol | Joback Method  |

# Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1005.68 | J/mol×K | 845.72          | Joback Method |
| cpg           | 911.14  | J/mol×K | 707.17          | Joback Method |
| cpg           | 931.80  | J/mol×K | 734.88          | Joback Method |
| cpg           | 951.55  | J/mol×K | 762.59          | Joback Method |
| cpg           | 970.43  | J/mol×K | 790.30          | Joback Method |
| cpg           | 988.46  | J/mol×K | 818.01          | Joback Method |
| cpg           | 1022.11 | J/mol×K | 873.43          | Joback Method |
| hvapt         | 70.90   | kJ/mol  | 605.50          | NIST Webbook  |

# Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 452.70 | K    | 0.30           | NIST Webbook |

# Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.53657e+01                   |
| Coeff. B                    | -5.59144e+03                  |
| Coeff. C                    | -1.16888e+02                  |
| Temperature range (K), min. | 487.72                        |
| Temperature range (K), max. | 673.02                        |

# Sources

|                 |                                                                                                                       |
|-----------------|-----------------------------------------------------------------------------------------------------------------------|
| 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> |

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1120496&Units=SI>

The Yaws Handbook of Vapor

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Pressure:

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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>hvapt:</b>   | Enthalpy of vaporization at a given temperature |
| <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>pvap:</b>    | Vapor pressure                                  |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tbrp:</b>    | Boiling point at reduced pressure               |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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