

# 1-Octanamine, n-octyl-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Di-n-octylamine<br>Dioctylamine<br>N-n-Octyl-n-octylamine<br>Rc 5632<br>di-Normal-octylamine |
| <b>Inchi:</b>               | InChI=1S/C16H35N/c1-3-5-7-9-11-13-15-17-16-14-12-10-8-6-4-2/h17H,3-16H2,1-2H3                |
| <b>InchiKey:</b>            | LAWOZCWGWDVVSU-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C16H35N  |
| <b>SMILES:</b>              | CCCCCCCCNCCCCCCCC  |
| <b>Mol. weight [g/mol]:</b> | 241.46   |
| <b>CAS:</b>                 | 1120-48-5  |

## Physical Properties

| Property code | Value            | Unit   | Source         |
|---------------|------------------|--------|----------------|
| chl           | -10890.90 ± 1.60 | kJ/mol | NIST Webbook   |
| gf            | 173.23           | kJ/mol | Joback Method  |
| hf            | -320.20 ± 2.30   | kJ/mol | NIST Webbook   |
| hfl           | -407.30 ± 1.90   | kJ/mol | NIST Webbook   |
| hfus          | 42.29            | kJ/mol | Joback Method  |
| hvap          | 87.10            | kJ/mol | NIST Webbook   |
| hvap          | 87.10 ± 1.30     | kJ/mol | NIST Webbook   |
| hvap          | 87.10 ± 1.30     | kJ/mol | NIST Webbook   |
| log10ws       | -5.71            |        | Crippen Method |
| logp          | 5.297            |        | Crippen Method |
| mvol          | 246.280          | ml/mol | McGowan Method |
| pc            | 1260.00 ± 300.00 | kPa    | NIST Webbook   |
| rhoc          | 220.93 ± 20.04   | kg/m3  | NIST Webbook   |
| tb            | 570.65 ± 7.00    | K      | NIST Webbook   |
| tb            | 570.70           | K      | NIST Webbook   |
| tc            | 734.00 ± 3.00    | K      | NIST Webbook   |
| tf            | 296.65 ± 1.40    | K      | NIST Webbook   |
| tf            | 283.45 ± 2.00    | K      | NIST Webbook   |
| tf            | 287.75 ± 0.50    | K      | NIST Webbook   |
| tf            | 309.65 ± 5.00    | K      | NIST Webbook   |
| tf            | 309.15 ± 5.00    | K      | NIST Webbook   |
| tf            | 287.65 ± 2.00    | K      | NIST Webbook   |
| tf            | 308.15 ± 5.00    | K      | NIST Webbook   |

|    |               |                      |               |
|----|---------------|----------------------|---------------|
| tf | 307.15 ± 5.00 | K                    | NIST Webbook  |
| tf | 287.77 ± 0.30 | K                    | NIST Webbook  |
| vc | 0.967         | m <sup>3</sup> /kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source  |
|---------------|--------|---------|-----------------|---|
| cpg           | 677.16 | J/mol×K | 615.65          | Joback Method   |
| cpg           | 696.09 | J/mol×K | 642.74          | Joback Method   |
| cpg           | 714.25 | J/mol×K | 669.83          | Joback Method   |
| cpg           | 731.65 | J/mol×K | 696.91          | Joback Method   |
| cpg           | 748.31 | J/mol×K | 724.00          | Joback Method   |
| cpg           | 764.27 | J/mol×K | 751.09          | Joback Method   |
| cpg           | 779.55 | J/mol×K | 778.18          | Joback Method   |
| cpl           | 507.20 | J/mol×K | 298.15          | NIST Webbook  |
| hvapt         | 92.60  | kJ/mol  | 298.15          | The vaporization enthalpy and vapor pressure of S (+)-methamphetamine at T = 298.15 K by correlation gas chromatography |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.66287e+01                   |
| Coeff. B                    | -5.62189e+03                  |
| Coeff. C                    | -1.02615e+02                  |
| Temperature range (K), min. | 446.65                        |
| Temperature range (K), max. | 599.37                        |

## Sources

|   |   |
|---|---|
| <b>NIST Webbook:</b>  | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1120485&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1120485&amp;Units=SI</a>   |
| <b>The Yaws Handbook of Vapor Pressure:</b>   | <a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a> |
| <b>Crippen Method:</b>  | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>The vaporization enthalpy and vapor pressure of S (+)-methamphetamine at 298.15 K by correlation gas chromatography:</b> | <a href="https://www.doi.org/10.1016/j.jct.2013.08.005">https://www.doi.org/10.1016/j.jct.2013.08.005</a>   |
| <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>   |

## Legend

|                 |   |
|-----------------|---|
| <b>chl:</b>     | Standard liquid enthalpy of combustion                    |
| <b>cpg:</b>     | Ideal gas heat capacity                                   |
| <b>cpl:</b>     | Liquid phase heat capacity                                |
| <b>gf:</b>      | Standard Gibbs free energy of formation                   |
| <b>hf:</b>      | Enthalpy of formation at standard conditions              |
| <b>hfl:</b>     | Liquid phase 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>rhoc:</b>    | Critical density  |
| <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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