# 1-Octanamine, N-methyl-N-octyl-

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|---|---|
| **Other names:** | Di(octyl)methylamine |
| | N,N-Dioctylmethylamine |
| | N-Methyldi-n-octylamine |
| | N-Methyldioctylamine |
| | methyldioctylamine |
| **Inchi:** | InChI=1S/C17H37N/c1-4-6-8-10-12-14-16-18(3)17-15-13-11-9-7-5-2/h4-17H2,1-3H3 |
| **InchiKey:** | YJLYANLCNIKXMG-UHFFFAOYSA-N |
| **Formula:** | C17H37N |
| **SMILES:** | CCCCCCCCN(C)CCCCCCCC |
| **Mol. weight [g/mol]:** | 255.48 |
| **CAS:** | 4455-26-9 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 203.04 | kJ/mol | Joback Method |
| hf | -326.68 | kJ/mol | Joback Method |
| hfus | 42.81 | kJ/mol | Joback Method |
| hvap | 55.48 | kJ/mol | Joback Method |
| log10ws | -5.51 | | Crippen Method |
| logp | 5.639 | | Crippen Method |
| mcvol | 260.370 | ml/mol | McGowan Method |
| pc | 1229.42 | kPa | Joback Method |
| ripol | 1770.00 | | NIST Webbook |
| tb | 600.80 | K | Joback Method |
| tc | 758.95 | K | Joback Method |
| tf | 313.82 | K | Joback Method |
| vc | 1.006 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 707.48 | J/mol×K | 600.80 | Joback Method |
| cpg | 727.42 | J/mol×K | 627.16 | Joback Method |
| cpg | 746.55 | J/mol×K | 653.52 | Joback Method |

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|---|---|---|---|---|
| cpg | 764.89 | J/mol×K | 679.87 | Joback Method |
| cpg | 782.48 | J/mol×K | 706.23 | Joback Method |
| cpg | 799.33 | J/mol×K | 732.59 | Joback Method |
| cpg | 815.46 | J/mol×K | 758.95 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.76453e+01 |
| Coeff. B | -6.07255e+03 |
| Coeff. C | -1.05712e+02 |
| Temperature range (K), min. | 455.56 |
| Temperature range (K), max. | 598.06 |

# Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C4455269&Units=SI

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

# Legend

**cpg:** Ideal gas heat capacity

**gf:** Standard Gibbs free energy of formation

**hf:** Enthalpy of formation at standard conditions

**hfus:** Enthalpy of fusion at standard conditions

**hvap:** Enthalpy of vaporization at standard conditions

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

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|---|---|
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |