

# Ethanol, 2-[bis(1-methylethyl)amino]-

|                      |                                                             |
|----------------------|-------------------------------------------------------------|
| Other names:         | 2-(Diisopropylamino)ethanol                                 |
|                      | 2-(Diisopropylamino)ethyl alcohol                           |
|                      | Diisopropylethanolamine                                     |
|                      | Ethanol, 2-(diisopropylamino)-                              |
|                      | Ethanol, diisopropylamino-                                  |
|                      | N,N-Diisopropylaminoethanol                                 |
|                      | N,N-Diisopropylethanolamine                                 |
|                      | NSC 45475                                                   |
| Inchi:               | UN 2825                                                     |
|                      | InChI=1S/C8H19NO/c1-7(2)9(5-6-10)8(3)4/h7-8,10H,5-6H2,1-4H3 |
|                      | ZYWUVGFIXPNBDL-UHFFFAOYSA-N                                 |
|                      |                                                             |
|                      |                                                             |
|                      |                                                             |
|                      |                                                             |
|                      |                                                             |
| InchiKey:            |                                                             |
| Formula:             | C8H19NO                                                     |
| SMILES:              | CC(C)N(CCO)C(C)C                                            |
| Mol. weight [g/mol]: | 145.25                                                      |
| CAS:                 | 96-80-0                                                     |

## Physical Properties

| Property code | Value         | Unit   | Source             |
|---------------|---------------|--------|--------------------|
| hfus          | 16.54         | kJ/mol | Joback Method      |
| hvap          | 59.30         | kJ/mol | Cheméo Relay (1.0) |
| ie            | 7.77          | eV     | Cheméo Relay (1.0) |
| logp          | 1.098         |        | Crippen Method     |
| mcvol         | 139.430       | ml/mol | McGowan Method     |
| pc            | 2829.33       | kPa    | Joback Method      |
| tb            | 463.20        | K      | NIST Webbook       |
| tf            | 233.90 ± 0.60 | K      | NIST Webbook       |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 323.15 | J/mol×K | 486.18          | Joback Method |
| cpg           | 336.07 | J/mol×K | 513.65          | Joback Method |
| cpg           | 348.45 | J/mol×K | 541.11          | Joback Method |
| cpg           | 360.30 | J/mol×K | 568.58          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 371.64 | J/mol×K | 596.05 | Joback Method |
| cpg | 382.49 | J/mol×K | 623.51 | Joback Method |
| cpg | 392.86 | J/mol×K | 650.98 | Joback Method |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.61053e+01                   |
| Coeff. B                    | -4.51777e+03                  |
| Coeff. C                    | -6.99060e+01                  |
| Temperature range (K), min. | 355.52                        |
| Temperature range (K), max. | 488.46                        |

## 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):            |                                                                                                                                                                                         |
| The Yaws Handbook of Vapor Pressure: | <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> |
| NIST Webbook:                        | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C96800&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C96800&amp;Units=SI</a>                                                 |
| Joback Method:                       | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                                                                   |

## Legend

|        |                                                 |
|--------|-------------------------------------------------|
| cpg:   | Ideal gas heat capacity                         |
| hfus:  | Enthalpy of fusion at standard conditions       |
| hvap:  | Enthalpy of vaporization at standard conditions |
| ie:    | Ionization energy                               |
| logp:  | Octanol/Water partition coefficient             |
| mcvol: | McGowan's characteristic volume                 |
| pc:    | Critical Pressure                               |

**pvap:** Vapor pressure  
**tb:** Normal Boiling Point Temperature  
**tf:** Normal melting (fusion) point

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