# 2-(isobutylamino)ethanol

**Inchi:** InChI=1S/C6H15NO/c1-6(2)5-7-3-4-8/h6-8H,3-5H2,1-2H3
**InchiKey:** VJWZYGQIJWDACM-UHFFFAOYSA-N
**Formula:** C6H15NO
**SMILES:** CC(C)CNCCO
**Mol. weight [g/mol]:** 117.19
**CAS:** 17091-40-6

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.6346 | | Cheméo Relay (1.0) |
| hf | -296.32 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 16.96 | kJ/mol | Joback Method |
| hvap | 62.55 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.48 | eV | Cheméo Relay (1.0) |
| logp | 0.224 | | Crippen Method |
| mcvol | 111.250 | ml/mol | McGowan Method |
| pc | 3538.87 | kPa | Joback Method |
| tb | 451.72 | K | Cheméo Relay (1.0) |
| tc | 609.27 | K | Cheméo Relay (1.0) |
| tf | 259.05 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 250.66 | J/mol×K | 478.59 | Joback Method |
| cpg | 261.02 | J/mol×K | 506.65 | Joback Method |
| cpg | 270.96 | J/mol×K | 534.72 | Joback Method |
| cpg | 280.50 | J/mol×K | 562.78 | Joback Method |
| cpg | 289.65 | J/mol×K | 590.84 | Joback Method |
| cpg | 298.41 | J/mol×K | 618.90 | Joback Method |
| cpg | 306.80 | J/mol×K | 646.97 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.43302e+01 |
| Coeff. B | -4.07673e+03 |
| Coeff. C | -7.24080e+01 |
| Temperature range (K), min. | 362.72 |
| Temperature range (K), max. | 524.44 |

# Sources

**Cheméo Relay (1.0, beta):**

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

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

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

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

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

**Cheméo Relay (1.0):**

# Legend

**af:** Acentric Factor
**cpg:** Ideal gas heat capacity
**hf:** Enthalpy of formation at standard conditions
**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
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point