

# Isobutyramide, N-dodecyl-

**Inchi:** InChI=1S/C16H33NO/c1-4-5-6-7-8-9-10-11-12-13-14-17-16(18)15(2)3/h15H,4-14H2,1-3H  
**InchiKey:** SVMMPBRZLZKBN-UHFFFAOYSA-N  
**Formula:** C16H33NO  
**SMILES:** CCCCCCCCCCN=C(O)C(C)C  
**Mol. weight [g/mol]:** 255.44

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | -458.65 | kJ/mol | Joback Method  |
| hvap          | 70.90   | kJ/mol | Joback Method  |
| log10ws       | -5.26   |        | Crippen Method |
| logp          | 5.520   |        | Crippen Method |
| mcvol         | 247.850 | ml/mol | McGowan Method |
| pc            | 1318.48 | kPa    | Joback Method  |
| rinpol        | 1998.00 |        | NIST Webbook   |
| rinpol        | 1998.00 |        | NIST Webbook   |
| tb            | 733.78  | K      | Joback Method  |
| tc            | 910.55  | K      | Joback Method  |

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/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=U407098&Units=SI>

## Legend

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

|                 |                                     |
|-----------------|-------------------------------------|
| <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>rinpol:</b>  | Non-polar retention indices         |
| <b>tb:</b>      | Normal Boiling Point Temperature    |
| <b>tc:</b>      | Critical Temperature                |

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