# Isophthalic acid, diamide, N,N'-dibutyl-

**Inchi:** InChI=1S/C16H24N2O2/c1-3-5-10-17-15(19)13-8-7-9-14(12-13)16(20)18-11-6-4-2/h7-9,1
**InchiKey:** UEUJQJBBZXOQII-UHFFFAOYSA-N
**Formula:** C16H24N2O2
**SMILES:** CCCCNC(=O)c1cccc(C(=O)NCCCC)c1
**Mol. weight [g/mol]:** 276.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 107.56 | kJ/mol | Joback Method |
| hf | -266.73 | kJ/mol | Joback Method |
| hfus | 44.24 | kJ/mol | Joback Method |
| hvap | 80.51 | kJ/mol | Joback Method |
| log10ws | -4.67 | | Crippen Method |
| logp | 2.746 | | Crippen Method |
| mcvol | 235.640 | ml/mol | McGowan Method |
| pc | 1913.58 | kPa | Joback Method |
| rinpol | 2746.00 | | NIST Webbook |
| rinpol | 2746.00 | | NIST Webbook |
| tb | 805.22 | K | Joback Method |
| tc | 1011.68 | K | Joback Method |
| tf | 514.20 | K | Joback Method |
| vc | 0.905 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 705.19 | J/mol×K | 805.22 | Joback Method |
| cpg | 719.66 | J/mol×K | 839.63 | Joback Method |
| cpg | 733.17 | J/mol×K | 874.04 | Joback Method |
| cpg | 745.75 | J/mol×K | 908.45 | Joback Method |
| cpg | 757.44 | J/mol×K | 942.86 | Joback Method |
| cpg | 768.30 | J/mol×K | 977.27 | Joback Method |
| cpg | 778.37 | J/mol×K | 1011.68 | Joback Method |

# Sources

| | |
|---|---|
| **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=U345813&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |