# [2-[(2-amino-2-oxoethyl)amino]-2-oxoethyl] benzoate

**Inchi:** InChI=1S/C11H12N2O4/c12-9(14)6-13-10(15)7-17-11(16)8-4-2-1-3-5-8/h1-5H,6-7H2,(H2

**InchiKey:** XYGUXAGVJDBSBP-UHFFFAOYSA-N

**Formula:** C11H12N2O4

**SMILES:** NC(=O)CNC(=O)COC(=O)c1ccccc1

**Mol. weight [g/mol]:** 236.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -181.77 | kJ/mol | Joback Method |
| hf | -416.54 | kJ/mol | Joback Method |
| hfus | 34.57 | kJ/mol | Joback Method |
| hvap | 82.08 | kJ/mol | Joback Method |
| log10ws | -1.50 | | Aqueous Solubility Prediction Method |
| logp | -0.555 | | Crippen Method |
| mcvol | 172.630 | ml/mol | McGowan Method |
| pc | 3456.14 | kPa | Joback Method |
| tb | 784.49 | K | Joback Method |
| tc | 1012.42 | K | Joback Method |
| tf | 424.65 | K | Aqueous Solubility Prediction Method |
| vc | 0.643 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 479.91 | J/mol×K | 784.49 | Joback Method |
| cpg | 490.25 | J/mol×K | 822.48 | Joback Method |
| cpg | 499.66 | J/mol×K | 860.47 | Joback Method |
| cpg | 508.17 | J/mol×K | 898.46 | Joback Method |
| cpg | 515.81 | J/mol×K | 936.45 | Joback Method |
| cpg | 522.61 | J/mol×K | 974.43 | Joback Method |
| cpg | 528.59 | J/mol×K | 1012.42 | Joback Method |

# Sources

| | |
|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |