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

**Inchi:** InChI=1S/C15H21NO3/c1-3-10-16(11-4-2)14(17)12-19-15(18)13-8-6-5-7-9-13/h5-9H,3-4
**InchiKey:** COTRONQEHWUCRV-UHFFFAOYSA-N
**Formula:** C15H21NO3
**SMILES:** CCCN(CCC)C(=O)COC(=O)c1ccccc1
**Mol. weight [g/mol]:** 263.34

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -64.23 | kJ/mol | Joback Method |
| hf | -406.25 | kJ/mol | Joback Method |
| hfus | 36.05 | kJ/mol | Joback Method |
| hvap | 69.20 | kJ/mol | Joback Method |
| log10ws | -2.38 | | Aqueous Solubility Prediction Method |
| logp | 2.492 | | Crippen Method |
| mcvol | 217.440 | ml/mol | McGowan Method |
| pc | 2029.06 | kPa | Joback Method |
| tb | 711.88 | K | Joback Method |
| tc | 914.00 | K | Joback Method |
| tf | 439.79 | K | Joback Method |
| vc | 0.816 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 606.84 | J/mol×K | 711.88 | Joback Method |
| cpg | 622.25 | J/mol×K | 745.57 | Joback Method |
| cpg | 636.67 | J/mol×K | 779.25 | Joback Method |
| cpg | 650.13 | J/mol×K | 812.94 | Joback Method |
| cpg | 662.69 | J/mol×K | 846.63 | Joback Method |
| cpg | 674.36 | J/mol×K | 880.32 | Joback Method |
| cpg | 685.18 | J/mol×K | 914.00 | Joback Method |

# Sources

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

# Legend

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|---|---|
| **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 |