# 5-ethyl-5-octyl-1,3-diazinane-2,4,6-trione

**Inchi:** InChI=1S/C14H24N2O3/c1-3-5-6-7-8-9-10-14(4-2)11(17)15-13(19)16-12(14)18/h3-10H2
**InchiKey:** NTYYDJWPKCQQIB-UHFFFAOYSA-N
**Formula:** C14H24N2O3
**SMILES:** CCCCCCCCC1(CC)C(=O)NC(=O)NC1=O
**Mol. weight [g/mol]:** 268.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -106.39 | kJ/mol | Joback Method |
| hf | -600.21 | kJ/mol | Joback Method |
| hfus | 35.26 | kJ/mol | Joback Method |
| hvap | 72.29 | kJ/mol | Joback Method |
| log10ws | -3.94 | | Aqueous and cosolvent solubility data for drug-like organic compounds |
| logp | 2.499 | | Crippen Method |
| mcvol | 221.930 | ml/mol | McGowan Method |
| pc | 2149.31 | kPa | Joback Method |
| tb | 840.07 | K | Joback Method |
| tc | 1074.84 | K | Joback Method |
| tf | 693.54 | K | Joback Method |
| vc | 0.846 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 722.26 | J/mol×K | 840.07 | Joback Method |
| cpg | 741.38 | J/mol×K | 879.20 | Joback Method |
| cpg | 759.44 | J/mol×K | 918.33 | Joback Method |
| cpg | 776.47 | J/mol×K | 957.46 | Joback Method |
| cpg | 792.49 | J/mol×K | 996.59 | Joback Method |
| cpg | 807.51 | J/mol×K | 1035.71 | Joback Method |
| cpg | 821.56 | J/mol×K | 1074.84 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Aqueous and cosolvent solubility data for drug-like organic compounds:** | https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/ |

# 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 |