# (E)-Nuciferyl isobutyrate

**Inchi:** InChI=1S/C19H28O2/c1-15(2)19(20)21-14-17(4)8-6-5-7-9-18-12-10-16(3)11-13-18/h8,10
**InchiKey:** PNFRTFPRRKETBY-CAOOACKPSA-N
**Formula:** C19H28O2
**SMILES:** CC(=CCCCCc1ccc(C)cc1)COC(=O)C(C)C
**Mol. weight [g/mol]:** 288.42

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 47.19 | kJ/mol | Joback Method |
| hf | -353.08 | kJ/mol | Joback Method |
| hfus | 36.77 | kJ/mol | Joback Method |
| hvap | 69.63 | kJ/mol | Joback Method |
| log10ws | -5.41 | | Crippen Method |
| logp | 4.853 | | Crippen Method |
| mcvol | 257.950 | ml/mol | McGowan Method |
| pc | 1462.37 | kPa | Joback Method |
| rinpol | 1975.00 | | NIST Webbook |
| rinpol | 1975.00 | | NIST Webbook |
| tb | 745.67 | K | Joback Method |
| tc | 948.22 | K | Joback Method |
| tf | 380.95 | K | Joback Method |
| vc | 0.991 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 744.16 | J/mol×K | 745.67 | Joback Method |
| cpg | 762.09 | J/mol×K | 779.43 | Joback Method |
| cpg | 778.95 | J/mol×K | 813.19 | Joback Method |
| cpg | 794.80 | J/mol×K | 846.94 | Joback Method |
| cpg | 809.68 | J/mol×K | 880.70 | Joback Method |
| cpg | 823.64 | J/mol×K | 914.46 | Joback Method |
| cpg | 836.72 | J/mol×K | 948.22 | Joback Method |

# Sources

| | |
|---|---|
| **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=R233073&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |