# 2-(Octyloxycarbonyl)benzoic acid

**Other names:** 2-(Octyloxycarbonyl)benzoic acid
**Inchi:** InChI=1S/C16H22O4/c1-2-3-4-5-6-9-12-20-16(19)14-11-8-7-10-13(14)15(17)18/h7-8,10-
**InchiKey:** PKIYFBICNICNGJ-UHFFFAOYSA-N
**Formula:** C16H22O4
**SMILES:** CCCCCCCCOC(=O)c1ccccc1C(=O)O
**Mol. weight [g/mol]:** 278.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 1.0322 | | Cheméo Relay (1.0) |
| hf | -765.05 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 39.32 | kJ/mol | Joback Method |
| hvap | 109.70 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.29 | eV | Cheméo Relay (1.0) |
| log10ws | -4.58 | | Cheméo Relay (1.0) |
| logp | 3.902 | | Crippen Method |
| mcvol | 227.420 | ml/mol | McGowan Method |
| pc | 1998.33 | kPa | Joback Method |
| rinpol | 2236.00 | | NIST Webbook |
| rinpol | 2236.00 | | NIST Webbook |
| tb | 615.22 | K | Cheméo Relay (1.0) |
| tc | 851.09 | K | Cheméo Relay (1.0) |
| tf | 347.63 | K | Cheméo Relay (1.0) |
| vc | 0.842 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 678.76 | J/mol×K | 819.48 | Joback Method |
| cpg | 691.54 | J/mol×K | 852.53 | Joback Method |
| cpg | 703.46 | J/mol×K | 885.57 | Joback Method |
| cpg | 714.54 | J/mol×K | 918.62 | Joback Method |
| cpg | 724.81 | J/mol×K | 951.66 | Joback Method |
| cpg | 734.30 | J/mol×K | 984.71 | Joback Method |

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|---|---|---|---|---|
| cpg | 743.02 | J/mol×K | 1017.75 | Joback Method |
| dvisc | 0.0006051 | Pa×s | 491.93 | Joback Method |
| dvisc | 0.0002614 | Pa×s | 546.52 | Joback Method |
| dvisc | 0.0001315 | Pa×s | 601.11 | Joback Method |
| dvisc | 0.0000742 | Pa×s | 655.70 | Joback Method |
| dvisc | 0.0000457 | Pa×s | 710.30 | Joback Method |
| dvisc | 0.0000302 | Pa×s | 764.89 | Joback Method |
| dvisc | 0.0000211 | Pa×s | 819.48 | Joback Method |

# Sources

| | |
|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C5393191&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **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 |