# (±)-2-octyl hydrogen phthalate

**Other names:** 2-((Octan-2-yloxy)carbonyl)benzoic acid
**Inchi:** InChI=1S/C16H22O4/c1-3-4-5-6-9-12(2)20-16(19)14-11-8-7-10-13(14)15(17)18/h7-8,10-
**InchiKey:** DUJBEEUYBSLMGM-UHFFFAOYSA-N
**Formula:** C16H22O4
**SMILES:** CCCCCCC(C)OC(=O)c1ccccc1C(=O)O
**Mol. weight [g/mol]:** 278.34
**CAS:** 68296-97-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -315.48 | kJ/mol | Joback Method |
| hf | -663.40 | kJ/mol | Joback Method |
| hfus | 35.80 | kJ/mol | Joback Method |
| hvap | 86.34 | kJ/mol | Joback Method |
| log10ws | -4.82 | | Crippen Method |
| logp | 3.901 | | Crippen Method |
| mcvol | 227.420 | ml/mol | McGowan Method |
| pc | 2012.70 | kPa | Joback Method |
| rinpol | 2143.00 | | NIST Webbook |
| rinpol | 2143.00 | | NIST Webbook |
| tb | 819.04 | K | Joback Method |
| tc | 1019.27 | K | Joback Method |
| tf | 476.93 | K | Joback Method |
| vc | 0.867 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 679.33 | J/mol×K | 819.04 | Joback Method |
| cpg | 735.19 | J/mol×K | 985.90 | Joback Method |
| cpg | 725.69 | J/mol×K | 952.52 | Joback Method |
| cpg | 715.38 | J/mol×K | 919.15 | Joback Method |
| cpg | 704.24 | J/mol×K | 885.78 | Joback Method |
| cpg | 692.23 | J/mol×K | 852.41 | Joback Method |

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|---|---|---|---|---|
| cpg | 743.90 | J/mol×K | 1019.27 | Joback Method |
| dvisc | 0.0000193 | Pa×s | 819.04 | Joback Method |
| dvisc | 0.0000283 | Pa×s | 762.02 | Joback Method |
| dvisc | 0.0000441 | Pa×s | 705.00 | Joback Method |
| dvisc | 0.0000742 | Pa×s | 647.99 | Joback Method |
| dvisc | 0.0001380 | Pa×s | 590.97 | Joback Method |
| dvisc | 0.0002933 | Pa×s | 533.95 | Joback Method |
| dvisc | 0.0007462 | Pa×s | 476.93 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C68296979&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# Legend

**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**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

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