# 3(2H)-Furanone, 5-methyl-2-octyl-

| | |
|---|---|
| **Other names:** | 2,3-Dihydro-2-n-octyl-5-methyl-furan-3-one |
| | 2,3-Dihydro-5-methyl-2-n-octylfuran-3-one |
| | 2H-Furan-3-one, 5-methyl-2-octyl |
| **Inchi:** | InChI=1S/C13H22O2/c1-3-4-5-6-7-8-9-13-12(14)10-11(2)15-13/h10,13H,3-9H2,1-2H3 |
| **InchiKey:** | ZLLDSWALGJWTSW-UHFFFAOYSA-N |
| **Formula:** | C13H22O2 |
| **SMILES:** | CCCCCCCCC1OC(C)=CC1=O |
| **Mol. weight [g/mol]:** | 210.31 |
| **CAS:** | 57877-72-2 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -93.25 | kJ/mol | Joback Method |
| hf | -474.56 | kJ/mol | Joback Method |
| hfus | 31.68 | kJ/mol | Joback Method |
| hvap | 54.50 | kJ/mol | Joback Method |
| log10ws | -3.99 | | Crippen Method |
| logp | 3.609 | | Crippen Method |
| mcvol | 186.310 | ml/mol | McGowan Method |
| pc | 1994.77 | kPa | Joback Method |
| rinpol | 1626.00 | | NIST Webbook |
| rinpol | 1652.80 | | NIST Webbook |
| rinpol | 1619.00 | | NIST Webbook |
| rinpol | 1622.00 | | NIST Webbook |
| rinpol | 1631.00 | | NIST Webbook |
| rinpol | 1626.00 | | NIST Webbook |
| rinpol | 1652.80 | | NIST Webbook |
| tb | 611.03 | K | Joback Method |
| tc | 809.57 | K | Joback Method |
| tf | 355.24 | K | Joback Method |
| vc | 0.719 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 501.23 | J/mol×K | 611.03 | Joback Method |
| cpg | 519.02 | J/mol×K | 644.12 | Joback Method |
| cpg | 535.96 | J/mol×K | 677.21 | Joback Method |
| cpg | 552.04 | J/mol×K | 710.30 | Joback Method |
| cpg | 567.27 | J/mol×K | 743.39 | Joback Method |
| cpg | 581.66 | J/mol×K | 776.48 | Joback Method |
| cpg | 595.23 | J/mol×K | 809.57 | Joback Method |

# Sources

**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
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C57877722&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# 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

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