# (Z)-3,7-Dimethylocta-2,6-dien-1-yl palmitate

**Inchi:** InChI=1S/C26H48O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-21-26(27)28-23-22-25(4)20
**InchiKey:** CRFQQFDSKWNZIZ-LVWGJNHUSA-N
**Formula:** C26H48O2
**SMILES:** CCCCCCCCCCCCCCCC(=O)OCC=C(C)CCC=C(C)C
**Mol. weight [g/mol]:** 392.66
**CAS:** 122569-17-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 77.46 | kJ/mol | Joback Method |
| hf | -609.91 | kJ/mol | Joback Method |
| hfus | 63.67 | kJ/mol | Joback Method |
| hvap | 82.70 | kJ/mol | Joback Method |
| log10ws | -9.28 | | Crippen Method |
| logp | 8.704 | | Crippen Method |
| mcvol | 376.040 | ml/mol | McGowan Method |
| pc | 791.71 | kPa | Joback Method |
| rinpol | 2726.20 | | NIST Webbook |
| rinpol | 2726.20 | | NIST Webbook |
| tb | 878.65 | K | Joback Method |
| tc | 1075.71 | K | Joback Method |
| tf | 416.86 | K | Joback Method |
| vc | 1.478 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1232.21 | J/mol×K | 878.65 | Joback Method |
| cpg | 1253.79 | J/mol×K | 911.49 | Joback Method |
| cpg | 1274.23 | J/mol×K | 944.34 | Joback Method |
| cpg | 1293.62 | J/mol×K | 977.18 | Joback Method |
| cpg | 1312.02 | J/mol×K | 1010.03 | Joback Method |
| cpg | 1329.51 | J/mol×K | 1042.87 | Joback Method |
| cpg | 1346.15 | J/mol×K | 1075.71 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C122569179&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 |

# 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 |