# Diethylmalonic acid, 2-formylphenyl octyl ester

**Inchi:** InChI=1S/C22H32O5/c1-4-7-8-9-10-13-16-26-20(24)22(5-2,6-3)21(25)27-19-15-12-11-14

**InchiKey:** ICJISCSIRIDCBK-UHFFFAOYSA-N

**Formula:** C22H32O5

**SMILES:** CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1C=O

**Mol. weight [g/mol]:** 376.49

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -327.38 | kJ/mol | Joback Method |
| hf | -856.28 | kJ/mol | Joback Method |
| hfus | 46.84 | kJ/mol | Joback Method |
| hvap | 91.24 | kJ/mol | Joback Method |
| log10ws | -6.09 | | Crippen Method |
| logp | 5.115 | | Crippen Method |
| mcvol | 313.530 | ml/mol | McGowan Method |
| pc | 1249.49 | kPa | Joback Method |
| rinpol | 2551.00 | | NIST Webbook |
| tb | 932.43 | K | Joback Method |
| tc | 1145.72 | K | Joback Method |
| tf | 565.38 | K | Joback Method |
| vc | 1.214 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1013.00 | J/mol×K | 932.43 | Joback Method |
| cpg | 1027.78 | J/mol×K | 967.98 | Joback Method |
| cpg | 1041.34 | J/mol×K | 1003.53 | Joback Method |
| cpg | 1053.74 | J/mol×K | 1039.08 | Joback Method |
| cpg | 1065.03 | J/mol×K | 1074.62 | Joback Method |
| cpg | 1075.26 | J/mol×K | 1110.17 | Joback Method |
| cpg | 1084.48 | J/mol×K | 1145.72 | Joback Method |
| dvisc | 0.0003973 | Pa×s | 565.38 | Joback Method |
| dvisc | 0.0002158 | Pa×s | 626.55 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001307 | Pa×s | 687.73 | Joback Method |
| dvisc | 0.0000859 | Pa×s | 748.90 | Joback Method |
| dvisc | 0.0000601 | Pa×s | 810.08 | Joback Method |
| dvisc | 0.0000443 | Pa×s | 871.25 | Joback Method |
| dvisc | 0.0000339 | Pa×s | 932.43 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U369953&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

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|---|---|
| **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 |