# Diethylmalonic acid, butyl 2-formylphenyl ester

**Inchi:** InChI=1S/C18H24O5/c1-4-7-12-22-16(20)18(5-2,6-3)17(21)23-15-11-9-8-10-14(15)13-19

**InchiKey:** AKVNWXXKNSODFJ-UHFFFAOYSA-N

**Formula:** C18H24O5

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

**Mol. weight [g/mol]:** 320.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -361.06 | kJ/mol | Joback Method |
| hf | -773.72 | kJ/mol | Joback Method |
| hfus | 36.48 | kJ/mol | Joback Method |
| hvap | 82.34 | kJ/mol | Joback Method |
| log10ws | -4.41 | | Crippen Method |
| logp | 3.554 | | Crippen Method |
| mcvol | 257.170 | ml/mol | McGowan Method |
| pc | 1672.79 | kPa | Joback Method |
| rinpol | 2159.00 | | NIST Webbook |
| tb | 840.91 | K | Joback Method |
| tc | 1051.29 | K | Joback Method |
| tf | 520.30 | K | Joback Method |
| vc | 0.990 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 778.64 | J/mol×K | 840.91 | Joback Method |
| cpg | 792.64 | J/mol×K | 875.97 | Joback Method |
| cpg | 805.55 | J/mol×K | 911.04 | Joback Method |
| cpg | 817.41 | J/mol×K | 946.10 | Joback Method |
| cpg | 828.26 | J/mol×K | 981.17 | Joback Method |
| cpg | 838.14 | J/mol×K | 1016.23 | Joback Method |
| cpg | 847.08 | J/mol×K | 1051.29 | Joback Method |
| dvisc | 0.0006246 | Pa×s | 520.30 | Joback Method |
| dvisc | 0.0003549 | Pa×s | 573.73 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002221 | Pa×s | 627.17 | Joback Method |
| dvisc | 0.0001496 | Pa×s | 680.61 | Joback Method |
| dvisc | 0.0001067 | Pa×s | 734.04 | Joback Method |
| dvisc | 0.0000797 | Pa×s | 787.47 | Joback Method |
| dvisc | 0.0000618 | Pa×s | 840.91 | Joback Method |

# Sources

**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

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U369949&Units=SI

# 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