# Diethylmalonic acid, 3-ethylphenyl propyl ester

**Inchi:** InChI=1S/C18H26O4/c1-5-12-21-16(19)18(7-3,8-4)17(20)22-15-11-9-10-14(6-2)13-15/h9
**InchiKey:** JDPATFBIHLWGHQ-UHFFFAOYSA-N
**Formula:** C18H26O4
**SMILES:** CCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(CC)c1
**Mol. weight [g/mol]:** 306.40

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -261.54 | kJ/mol | Joback Method |
| hf | -688.14 | kJ/mol | Joback Method |
| hfus | 34.19 | kJ/mol | Joback Method |
| hvap | 75.62 | kJ/mol | Joback Method |
| log10ws | -4.56 | | Crippen Method |
| logp | 3.914 | | Crippen Method |
| mcvol | 255.600 | ml/mol | McGowan Method |
| pc | 1575.95 | kPa | Joback Method |
| rinpol | 1959.00 | | NIST Webbook |
| rinpol | 1959.00 | | NIST Webbook |
| tb | 792.25 | K | Joback Method |
| tc | 998.90 | K | Joback Method |
| tf | 478.30 | K | Joback Method |
| vc | 0.973 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 762.82 | J/mol×K | 792.25 | Joback Method |
| cpg | 778.75 | J/mol×K | 826.69 | Joback Method |
| cpg | 793.58 | J/mol×K | 861.13 | Joback Method |
| cpg | 807.34 | J/mol×K | 895.58 | Joback Method |
| cpg | 820.07 | J/mol×K | 930.02 | Joback Method |
| cpg | 831.80 | J/mol×K | 964.46 | Joback Method |
| cpg | 842.58 | J/mol×K | 998.90 | Joback Method |
| dvisc | 0.0006763 | Pa×s | 478.30 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003670 | Pa×s | 530.62 | Joback Method |
| dvisc | 0.0002223 | Pa×s | 582.95 | Joback Method |
| dvisc | 0.0001462 | Pa×s | 635.27 | Joback Method |
| dvisc | 0.0001025 | Pa×s | 687.60 | Joback Method |
| dvisc | 0.0000756 | Pa×s | 739.92 | Joback Method |
| dvisc | 0.0000580 | Pa×s | 792.25 | 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=U370584&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 |