# 1-Naphthoic acid, 3-methylphenyl ester

**Inchi:** InChI=1S/C18H14O2/c1-13-6-4-9-15(12-13)20-18(19)17-11-5-8-14-7-2-3-10-16(14)17/h2
**InchiKey:** UQUNKEZAIBXBIQ-UHFFFAOYSA-N
**Formula:** C18H14O2
**SMILES:** Cc1cccc(OC(=O)c2cccc3ccccc23)c1
**Mol. weight [g/mol]:** 262.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 178.97 | kJ/mol | Joback Method |
| hf | -18.46 | kJ/mol | Joback Method |
| hfus | 29.49 | kJ/mol | Joback Method |
| hvap | 72.33 | kJ/mol | Joback Method |
| log10ws | -5.84 | | Crippen Method |
| logp | 4.367 | | Crippen Method |
| mcvol | 204.940 | ml/mol | McGowan Method |
| pc | 2443.48 | kPa | Joback Method |
| rinpol | 2312.00 | | NIST Webbook |
| rinpol | 2312.00 | | NIST Webbook |
| tb | 769.83 | K | Joback Method |
| tc | 1021.87 | K | Joback Method |
| tf | 475.36 | K | Joback Method |
| vc | 0.773 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 555.08 | J/mol×K | 769.83 | Joback Method |
| cpg | 569.74 | J/mol×K | 811.84 | Joback Method |
| cpg | 583.16 | J/mol×K | 853.84 | Joback Method |
| cpg | 595.43 | J/mol×K | 895.85 | Joback Method |
| cpg | 606.66 | J/mol×K | 937.86 | Joback Method |
| cpg | 616.95 | J/mol×K | 979.87 | Joback Method |
| cpg | 626.39 | J/mol×K | 1021.87 | Joback Method |
| dvisc | 0.0009517 | Pa×s | 475.36 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0006369 | Pa×s | 524.44 | Joback Method |
| dvisc | 0.0004565 | Pa×s | 573.52 | Joback Method |
| dvisc | 0.0003449 | Pa×s | 622.60 | Joback Method |
| dvisc | 0.0002714 | Pa×s | 671.67 | Joback Method |
| dvisc | 0.0002207 | Pa×s | 720.75 | Joback Method |
| dvisc | 0.0001843 | Pa×s | 769.83 | Joback Method |

# Sources

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|---|---|
| **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=U307823&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 |