# 1-Naphthaleneacetic acid, 3-chlorophenyl ester

**Inchi:** InChI=1S/C18H13ClO2/c19-15-8-4-9-16(12-15)21-18(20)11-14-7-3-6-13-5-1-2-10-17(13)

**InchiKey:** XNTAOMRNPHSFMO-UHFFFAOYSA-N

**Formula:** C18H13ClO2

**SMILES:** O=C(Cc1cccc2ccccc12)Oc1cccc(Cl)c1

**Mol. weight [g/mol]:** 296.75

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 167.04 | kJ/mol | Joback Method |
| hf | -34.20 | kJ/mol | Joback Method |
| hfus | 33.68 | kJ/mol | Joback Method |
| hvap | 76.72 | kJ/mol | Joback Method |
| log10ws | -5.89 | | Crippen Method |
| logp | 4.641 | | Crippen Method |
| mcvol | 217.180 | ml/mol | McGowan Method |
| pc | 2356.49 | kPa | Joback Method |
| rinpol | 3065.00 | | NIST Webbook |
| rinpol | 3065.00 | | NIST Webbook |
| tb | 807.26 | K | Joback Method |
| tc | 1061.03 | K | Joback Method |
| tf | 505.28 | K | Joback Method |
| vc | 0.823 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 578.01 | J/mol×K | 807.26 | Joback Method |
| cpg | 633.85 | J/mol×K | 1018.74 | Joback Method |
| cpg | 624.58 | J/mol×K | 976.44 | Joback Method |
| cpg | 614.47 | J/mol×K | 934.15 | Joback Method |
| cpg | 603.40 | J/mol×K | 891.85 | Joback Method |
| cpg | 591.29 | J/mol×K | 849.56 | Joback Method |
| cpg | 642.38 | J/mol×K | 1061.03 | Joback Method |
| dvisc | 0.0001699 | Pa×s | 807.26 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002038 | Pa×s | 756.93 | Joback Method |
| dvisc | 0.0002510 | Pa×s | 706.60 | Joback Method |
| dvisc | 0.0003191 | Pa×s | 656.27 | Joback Method |
| dvisc | 0.0004222 | Pa×s | 605.94 | Joback Method |
| dvisc | 0.0005876 | Pa×s | 555.61 | Joback Method |
| dvisc | 0.0008735 | Pa×s | 505.28 | Joback Method |

# Sources

| | |
|---|---|
| **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=U415051&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |