# 1-Naphthalenecarboxamide, N-(2-iodo-4-methylphenyl)-

**Inchi:** InChI=1S/C18H14INO/c1-12-9-10-17(16(19)11-12)20-18(21)15-8-4-6-13-5-2-3-7-14(13)1

**InchiKey:** NTNUZQYVQIVDHA-UHFFFAOYSA-N

**Formula:** C18H14INO

**SMILES:** Cc1ccc(NC(=O)c2cccc3ccccc23)c(I)c1

**Mol. weight [g/mol]:** 387.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 421.85 | kJ/mol | Joback Method |
| hf | 232.63 | kJ/mol | Joback Method |
| hfus | 37.41 | kJ/mol | Joback Method |
| hvap | 86.39 | kJ/mol | Joback Method |
| log10ws | -6.88 | | Crippen Method |
| logp | 5.005 | | Crippen Method |
| mcvol | 234.870 | ml/mol | McGowan Method |
| pc | 2426.65 | kPa | Joback Method |
| rinpol | 3023.00 | | NIST Webbook |
| tb | 895.70 | K | Joback Method |
| tc | 1169.94 | K | Joback Method |
| tf | 576.37 | K | Joback Method |
| vc | 0.878 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 619.30 | J/mol×K | 895.70 | Joback Method |
| cpg | 631.60 | J/mol×K | 941.41 | Joback Method |
| cpg | 643.01 | J/mol×K | 987.11 | Joback Method |
| cpg | 653.70 | J/mol×K | 1032.82 | Joback Method |
| cpg | 663.86 | J/mol×K | 1078.53 | Joback Method |
| cpg | 673.64 | J/mol×K | 1124.23 | Joback Method |
| cpg | 683.23 | J/mol×K | 1169.94 | Joback Method |

# Sources

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|---|---|
| **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=U307410&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |