# 2,6-Naphthalenedicarboxylic acid

**Other names:** 2,6-naphthalic acid
naphthalene-2,6-dicarboxylic acid
**Inchi:** InChI=1S/C12H8O4/c13-11(14)9-3-1-7-5-10(12(15)16)4-2-8(7)6-9/h1-6H,(H,13,14)(H,15,
**InchiKey:** RXOHFPCZGPKIRD-UHFFFAOYSA-N
**Formula:** C12H8O4
**SMILES:** O=C(O)c1ccc2cc(C(=O)O)ccc2c1
**Mol. weight [g/mol]:** 216.19
**CAS:** 1141-38-4

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -5095.19 ± 0.78 | kJ/mol | NIST Webbook |
| gf | -281.52 | kJ/mol | Joback Method |
| hf | -415.97 | kJ/mol | Joback Method |
| hfs | -770.25 ± 0.96 | kJ/mol | NIST Webbook |
| hfus | 28.49 | kJ/mol | Joback Method |
| hvap | 94.40 | kJ/mol | Joback Method |
| log10ws | -3.40 | | Crippen Method |
| logp | 2.236 | | Crippen Method |
| mcvol | 151.600 | ml/mol | McGowan Method |
| pc | 4362.63 | kPa | Joback Method |
| tb | 821.68 | K | Joback Method |
| tc | 1035.21 | K | Joback Method |
| tf | 530.66 | K | Joback Method |
| vc | 0.572 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 406.62 | J/mol×K | 821.68 | Joback Method |
| cpg | 413.86 | J/mol×K | 857.27 | Joback Method |
| cpg | 420.61 | J/mol×K | 892.86 | Joback Method |
| cpg | 426.90 | J/mol×K | 928.45 | Joback Method |
| cpg | 432.80 | J/mol×K | 964.03 | Joback Method |

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|---|---|---|---|---|
| cpg | 438.35 | J/mol×K | 999.62 | Joback Method |
| cpg | 443.61 | J/mol×K | 1035.21 | Joback Method |
| cps | 230.30 | J/mol×K | 298.15 | NIST Webbook |
| dvisc | 0.0004215 | Pa×s | 530.66 | Joback Method |
| dvisc | 0.0001913 | Pa×s | 579.16 | Joback Method |
| dvisc | 0.0000981 | Pa×s | 627.67 | Joback Method |
| dvisc | 0.0000554 | Pa×s | 676.17 | Joback Method |
| dvisc | 0.0000337 | Pa×s | 724.67 | Joback Method |
| dvisc | 0.0000219 | Pa×s | 773.18 | Joback Method |
| dvisc | 0.0000149 | Pa×s | 821.68 | 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=C1141384&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Thermodynamic Properties and Crystal Structures of the Adductive Crystallization with N,N-Dimethyl Acetamide and N-Methyl Pyrrolidone:** | https://www.doi.org/10.1021/je2009973 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **2,6-Naphthalenedicarboxylic Acid** | |

# Legend

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|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **cps:** | Solid phase heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |

**vc:** Critical Volume