# 1-Amino-2-bromo-4-p-toluidinoanthraquinone

**Other names:** 1-Amino-2-bromo-4-[(4-methylphenyl)amino]-9,10-anthraquinone
**Inchi:** InChI=1S/C21H15BrN2O2/c1-11-6-8-12(9-7-11)24-16-10-15(22)19(23)18-17(16)20(25)1
**InchiKey:** SPDRRRCQUXHHLH-UHFFFAOYSA-N
**Formula:** C21H15BrN2O2
**SMILES:** Cc1ccc(Nc2cc(Br)c(N)c3c2C(=O)c2ccccc2C3=O)cc1
**Mol. weight [g/mol]:** 407.26
**CAS:** 128-83-6

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 410.93 | kJ/mol | Joback Method |
| hf | 101.49 | kJ/mol | Joback Method |
| hfus | 43.70 | kJ/mol | Joback Method |
| hvap | 105.20 | kJ/mol | Joback Method |
| log10ws | -6.71 | | Crippen Method |
| logp | 4.859 | | Crippen Method |
| mcvol | 265.210 | ml/mol | McGowan Method |
| pc | 2540.49 | kPa | Joback Method |
| tb | 1121.44 | K | Joback Method |
| tc | 1407.71 | K | Joback Method |
| tf | 838.67 | K | Joback Method |
| vc | 0.994 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 808.99 | J/mol×K | 1121.44 | Joback Method |
| cpg | 817.77 | J/mol×K | 1169.15 | Joback Method |
| cpg | 825.30 | J/mol×K | 1216.86 | Joback Method |
| cpg | 831.70 | J/mol×K | 1264.57 | Joback Method |
| cpg | 837.07 | J/mol×K | 1312.29 | Joback Method |
| cpg | 841.49 | J/mol×K | 1360.00 | Joback Method |
| cpg | 845.08 | J/mol×K | 1407.71 | Joback Method |
| hsubt | 167.00 ± 6.00 | kJ/mol | 428.00 | NIST Webbook |

# Sources

| | |
|---|---|
| **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=C128836&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **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 |
| **hsubt:** | Enthalpy of sublimation at a given temperature |
| **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 |

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