# 1,5-DIAMINOANTHRAQUINONE

| | |
|---|---|
| **Other names:** | 9,10-Anthracenedione, 1,5-diamino- |
| | Anthraquinone, 1,5-diamino- |
| | C.I. Disperse Red II |
| | 1,5-Anthraquinonyldiamine |
| | 1,5-Daa |
| | 1,5-Diamino-9,10-anthraquinone |
| | 1,5-Diaminoanthrachinon |
| | NSC 63791 |
| | NSC 7213 |
| | Smoke Red F |
| **Inchi:** | InChI=1S/C14H10N2O2/c15-9-5-1-3-7-11(9)14(18)8-4-2-6-10(16)12(8)13(7)17/h1-6H,15 |
| **InchiKey:** | VWBVCOPVKXNMMZ-UHFFFAOYSA-N |
| **Formula:** | C14H10N2O2 |
| **SMILES:** | Nc1cccc2c1C(=O)c1cccc(N)c1C2=O |
| **Mol. weight [g/mol]:** | 238.25 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -85.93 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 27.12 | kJ/mol | Joback Method |
| ie | 7.70 | eV | Cheméo Relay (1.0) |
| log10ws | -3.93 | | Cheméo Relay (1.0) |
| logp | 1.626 | | Crippen Method |
| mcvol | 172.840 | ml/mol | McGowan Method |
| tb | 683.44 | K | Cheméo Relay (1.0) |
| tf | 525.39 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 507.63 | J/mol×K | 880.84 | Joback Method |
| cpg | 518.91 | J/mol×K | 927.66 | Joback Method |
| cpg | 528.94 | J/mol×K | 974.48 | Joback Method |
| cpg | 537.75 | J/mol×K | 1021.30 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 545.39 | J/mol×K | 1068.12 | Joback Method |
| cpg | 551.89 | J/mol×K | 1114.94 | Joback Method |
| cpg | 557.29 | J/mol×K | 1161.76 | Joback Method |
| hsubt | 118.50 ± 4.80 | kJ/mol | 416.00 | NIST Webbook |

# Sources

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C129442&Units=SI

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Cheméo Relay (1.0):**

# Legend

**cpg:** Ideal gas heat capacity
**hf:** Enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hsubt:** Enthalpy of sublimation at a given temperature
**ie:** Ionization energy
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**tb:** Normal Boiling Point Temperature
**tf:** Normal melting (fusion) point