# 2,1,3-Benzoxadiazole, 4,6-dinitro-, 1-oxide

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|---|---|
| **Other names:** | 2,1,3-Benzoxadiazole, 4,6-dinitro-, 1-oxide |
| | 4,6-Dinitrobenzofurazan 1-oxide |
| | 4,6-Dinitrobenzofurazan oxide |
| | 4,6-Dinitrobenzofuroxan |
| **Inchi:** | InChI=1S/C6H2N4O6/c11-8(12)3-1-4(9(13)14)6-5(2-3)10(15)16-7-6/h1-2H |
| **InchiKey:** | YHBBUAULQKLKMW-UHFFFAOYSA-N |
| **Formula:** | C6H2N4O6 |
| **SMILES:** | O=[N+]([O-])c1cc([N+](=O)[O-])c2no[n+]([O-])c2c1 |
| **Mol. weight [g/mol]:** | 226.10 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | 301.40 | kJ/mol | Cheméo Relay (1.0) |
| hvap | 90.82 | kJ/mol | Cheméo Relay (1.0) |
| ie | 10.34 | eV | Cheméo Relay (1.0) |
| log10ws | -3.11 | | Cheméo Relay (1.0) |
| logp | 0.278 | | Crippen Method |
| mcvol | 123.020 | ml/mol | McGowan Method |
| tf | 427.94 | K | Cheméo Relay (1.0) |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| hfust | 20.73 | kJ/mol | 452.70 | NIST Webbook |

# Sources

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|---|---|
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C5128289&Units=SI |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

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| **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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|---|---|
| **hf:** | Enthalpy of formation at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **tf:** | Normal melting (fusion) point |