

# Ammonium o-phthalate

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Other names:         | Ammonium o-phthalate                                                              |
| Inchi:               | InChI=1S/C8H6O4.2H3N/c9-7(10)5-3-1-2-4-6(5)8(11)12;/h1-4H,(H,9,10)(H,11,12);2*1H3 |
| InchiKey:            | CHCFOMQHQIQBLZ-UHFFFAOYSA-N                                                       |
| Formula:             | C8H12N2O4                                                                         |
| SMILES:              | O=C([O-])c1ccccc1C(=O)[O-].[NH4+].[NH4+]                                          |
| Mol. weight [g/mol]: | 200.19                                                                            |

## Physical Properties

| Property code | Value   | Unit   | Source                   |
|---------------|---------|--------|--------------------------|
| hf            | -661.68 | kJ/mol | Cheméo Relay (1.0)       |
| hvap          | 85.97   | kJ/mol | Cheméo Relay (1.0)       |
| ie            | 9.78    | eV     | Cheméo Relay (1.0)       |
| log10ws       | -2.16   |        | Cheméo Relay (1.0)       |
| pc            | 3391.17 | kPa    | Cheméo Relay (1.0, beta) |
| tb            | 554.43  | K      | Cheméo Relay (1.0)       |
| tc            | 689.52  | K      | Cheméo Relay (1.0)       |
| tf            | 482.89  | K      | Cheméo Relay (1.0)       |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source       |
|---------------|--------|---------|-----------------|--------------|
| cps           | 294.10 | J/mol×K | 323.00          | NIST Webbook |

## Sources

|                           |                                                                                                                                           |
|---------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C523240&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C523240&amp;Units=SI</a> |
| Cheméo Relay (1.0):       |                                                                                                                                           |
| Cheméo Relay (1.0, beta): |                                                                                                                                           |

# Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cps:</b>     | Solid phase heat capacity                       |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>ie:</b>      | Ionization energy                               |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>pc:</b>      | Critical Pressure                               |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |

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