

# 2,4,7-Trinitrofluorenone

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 9H-Fluoren-9-one, 2,4,7-trinitro-Fluoren-9-one, 2,4,7-trinitro-TNF<br>2,4,7-Trinitrofluoren-9-one<br>2,4,7-Trinitro-9-fluorenone |
| <b>Inchi:</b>               | InChI=1S/C13H5N3O7/c17-13-9-3-6(14(18)19)1-2-8(9)12-10(13)4-7(15(20)21)5-11(12)1   |
| <b>InchiKey:</b>            | VHQGURIJMF PBKS-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C13H5N3O7  |
| <b>SMILES:</b>              | O=C1c2cc([N+](=O)[O-])ccc2-c2c1cc([N+](=O)[O-])cc2[N+](=O)[O-]   |
| <b>Mol. weight [g/mol]:</b> | 315.19   |
| <b>CAS:</b>                 | 129-79-3   |

## Physical Properties

| Property code | Value         | Unit    | Source         |
|---------------|---------------|---------|----------------|
| gf            | 311.97        | kJ/mol  | Joback Method  |
| hf            | 39.54         | kJ/mol  | Joback Method  |
| hfus          | 50.42         | kJ/mol  | Joback Method  |
| hvap          | 106.29        | kJ/mol  | Joback Method  |
| log10ws       | -6.23         |         | Crippen Method |
| logp          | 2.623         |         | Crippen Method |
| mcvol         | 189.480       | ml/mol  | McGowan Method |
| pc            | 3480.65       | kPa     | Joback Method  |
| tb            | 1101.31       | K       | Joback Method  |
| tc            | 1405.24       | K       | Joback Method  |
| tf            | 449.00 ± 0.50 | K       | NIST Webbook   |
| tf            | 449.00 ± 0.30 | K       | NIST Webbook   |
| tf            | 448.15 ± 2.00 | K       | NIST Webbook   |
| vc            | 0.774         | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 598.21 | J/molxK | 1354.58         | Joback Method |
| cpg           | 561.97 | J/molxK | 1101.31         | Joback Method |

|       |        |         |         |               |
|-------|--------|---------|---------|---------------|
| cpg   | 569.58 | J/mol×K | 1151.96 | Joback Method |
| cpg   | 576.85 | J/mol×K | 1202.62 | Joback Method |
| cpg   | 583.94 | J/mol×K | 1253.27 | Joback Method |
| cpg   | 591.01 | J/mol×K | 1303.93 | Joback Method |
| cpg   | 605.71 | J/mol×K | 1405.24 | Joback Method |
| hfust | 23.50  | kJ/mol  | 449.20  | NIST Webbook  |

## Sources

|                        |   |
|------------------------|---|
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C129793&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C129793&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hfust:</b>   | Enthalpy of fusion at a given temperature       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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