# 9H-Fluorene, 2,7-dinitro-

**Other names:** Fluorene, 2,7-dinitro-
2,7-Dinitrofluorene
**Inchi:** InChI=1S/C13H8N2O4/c16-14(17)10-1-3-12-8(6-10)5-9-7-11(15(18)19)2-4-13(9)12/h1-4,
**InchiKey:** IHZCVUBSTYOFSJ-UHFFFAOYSA-N
**Formula:** C13H8N2O4
**SMILES:** O=[N+]([O-])c1ccc2c(c1)Cc1cc([N+](=O)[O-])ccc1-2
**Mol. weight [g/mol]:** 256.21
**CAS:** 5405-53-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 408.64 | kJ/mol | Joback Method |
| hf | 199.47 | kJ/mol | Joback Method |
| hfus | 39.94 | kJ/mol | Joback Method |
| hvap | 84.79 | kJ/mol | Joback Method |
| log10ws | -5.72 | | Crippen Method |
| logp | 3.074 | | Crippen Method |
| mcvol | 170.490 | ml/mol | McGowan Method |
| pc | 3352.86 | kPa | Joback Method |
| rinpol | 427.47 | | NIST Webbook |
| rinpol | 431.80 | | NIST Webbook |
| rinpol | 427.47 | | NIST Webbook |
| tb | 876.67 | K | Joback Method |
| tc | 1162.30 | K | Joback Method |
| tf | 655.63 | K | Joback Method |
| vc | 0.685 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 477.18 | J/mol×K | 876.67 | Joback Method |
| cpg | 487.43 | J/mol×K | 924.27 | Joback Method |
| cpg | 497.17 | J/mol×K | 971.88 | Joback Method |
| cpg | 506.63 | J/mol×K | 1019.48 | Joback Method |

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|---|---|---|---|---|
| cpg | 515.99 | J/mol×K | 1067.09 | Joback Method |
| cpg | 525.49 | J/mol×K | 1114.69 | Joback Method |
| cpg | 535.31 | J/mol×K | 1162.30 | Joback Method |

# Sources

| | |
|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **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=C5405538&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |