# Fluoranthene, 3-nitro-

**Other names:** 3-Nitrofluoranthene
4-Nitrofluoranthene
**Inchi:** InChI=1S/C16H9NO2/c18-17(19)15-9-8-13-11-5-2-1-4-10(11)12-6-3-7-14(15)16(12)13/h
**InchiKey:** PIHGQKMEAMSUNA-UHFFFAOYSA-N
**Formula:** C16H9NO2
**SMILES:** O=[N+]([O-])c1ccc2c3c(cccc13)-c1ccccc1-2
**Mol. weight [g/mol]:** 247.25
**CAS:** 892-21-7

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 517.10 | kJ/mol | Joback Method |
| hf | 345.54 | kJ/mol | Joback Method |
| hfus | 35.47 | kJ/mol | Joback Method |
| hvap | 76.35 | kJ/mol | Joback Method |
| log10ws | -7.38 | | Crippen Method |
| logp | 4.395 | | Crippen Method |
| mcvol | 175.880 | ml/mol | McGowan Method |
| pc | 3062.55 | kPa | Joback Method |
| rinpol | 413.24 | | NIST Webbook |
| rinpol | 419.80 | | NIST Webbook |
| rinpol | 423.90 | | NIST Webbook |
| rinpol | 411.89 | | NIST Webbook |
| rinpol | 412.45 | | NIST Webbook |
| rinpol | 412.45 | | NIST Webbook |
| rinpol | 2433.00 | | NIST Webbook |
| rinpol | 413.34 | | NIST Webbook |
| rinpol | 2433.00 | | NIST Webbook |
| rinpol | 413.33 | | NIST Webbook |
| rinpol | 411.89 | | NIST Webbook |
| rinpol | 413.34 | | NIST Webbook |
| rinpol | 423.90 | | NIST Webbook |
| tb | 808.18 | K | Joback Method |
| tc | 1082.43 | K | Joback Method |
| tf | 582.05 | K | Joback Method |
| vc | 0.702 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 473.39 | J/mol×K | 808.18 | Joback Method |
| cpg | 484.71 | J/mol×K | 853.89 | Joback Method |
| cpg | 495.53 | J/mol×K | 899.60 | Joback Method |
| cpg | 506.09 | J/mol×K | 945.31 | Joback Method |
| cpg | 516.66 | J/mol×K | 991.01 | Joback Method |
| cpg | 527.49 | J/mol×K | 1036.72 | Joback Method |
| cpg | 538.85 | J/mol×K | 1082.43 | Joback Method |
| hfust | 22.60 | kJ/mol | 435.00 | NIST Webbook |

# Sources

| | |
|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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=C892217&Units=SI |

# 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 |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **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 |

Latest version available from:
https://www.chemeo.com/cid/96-409-2/Fluoranthene-3-nitro.pdf
Generated by Cheméo on 2024-04-24 08:07:30.466512746 +0000 UTC m=+16235299.387090060.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.