# Phenanthrene, 2,4,6-trifluoro

**Inchi:** InChI=1S/C14H7F3/c15-10-4-3-8-1-2-9-5-11(16)7-13(17)14(9)12(8)6-10/h1-7H
**InchiKey:** MOWMOCXMCHFRQY-UHFFFAOYSA-N
**Formula:** C14H7F3
**SMILES:** Fc1cc(F)c2c(ccc3ccc(F)cc32)c1
**Mol. weight [g/mol]:** 232.20

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -230.24 | kJ/mol | Joback Method |
| hf | -347.83 | kJ/mol | Joback Method |
| hfus | 27.78 | kJ/mol | Joback Method |
| hvap | 52.51 | kJ/mol | Joback Method |
| log10ws | -6.08 | | Crippen Method |
| logp | 4.410 | | Crippen Method |
| mcvol | 150.750 | ml/mol | McGowan Method |
| pc | 2668.02 | kPa | Joback Method |
| rinpol | 1687.00 | | NIST Webbook |
| rinpol | 288.88 | | NIST Webbook |
| rinpol | 1679.00 | | NIST Webbook |
| rinpol | 288.88 | | NIST Webbook |
| rinpol | 288.87 | | NIST Webbook |
| rinpol | 1687.00 | | NIST Webbook |
| ripol | 280.76 | | NIST Webbook |
| ripol | 280.76 | | NIST Webbook |
| tb | 602.09 | K | Joback Method |
| tc | 822.85 | K | Joback Method |
| tf | 391.21 | K | Joback Method |
| vc | 0.610 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 356.26 | J/mol×K | 602.09 | Joback Method |
| cpg | 368.17 | J/mol×K | 638.88 | Joback Method |

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|---|---|---|---|---|
| cpg | 379.20 | J/mol×K | 675.68 | Joback Method |
| cpg | 389.43 | J/mol×K | 712.47 | Joback Method |
| cpg | 398.94 | J/mol×K | 749.26 | Joback Method |
| cpg | 407.80 | J/mol×K | 786.05 | Joback Method |
| cpg | 416.09 | J/mol×K | 822.85 | Joback Method |

# Sources

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|---|---|
| **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=R76135&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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |