# 6-Aminochrysene TFA

**Inchi:** InChI=1S/C20H12F3NO/c21-20(22,23)19(25)24-18-11-17-13-6-2-1-5-12(13)9-10-15(17)1

**InchiKey:** LJGJMCASWROFLL-UHFFFAOYSA-N

**Formula:** C20H12F3NO

**SMILES:** O=C(Nc1cc2c3ccccc3ccc2c2ccccc12)C(F)(F)F

**Mol. weight [g/mol]:** 339.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -100.13 | kJ/mol | Joback Method |
| hf | -336.99 | kJ/mol | Joback Method |
| hfus | 40.01 | kJ/mol | Joback Method |
| hvap | 78.73 | kJ/mol | Joback Method |
| log10ws | -7.75 | | Crippen Method |
| logp | 5.647 | | Crippen Method |
| mcvol | 227.380 | ml/mol | McGowan Method |
| pc | 2149.31 | kPa | Joback Method |
| rinpol | 443.06 | | NIST Webbook |
| tb | 854.18 | K | Joback Method |
| tc | 1091.34 | K | Joback Method |
| tf | 584.02 | K | Joback Method |
| vc | 0.897 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 658.72 | J/mol×K | 854.18 | Joback Method |
| cpg | 670.47 | J/mol×K | 893.71 | Joback Method |
| cpg | 681.65 | J/mol×K | 933.23 | Joback Method |
| cpg | 692.43 | J/mol×K | 972.76 | Joback Method |
| cpg | 703.02 | J/mol×K | 1012.28 | Joback Method |
| cpg | 713.60 | J/mol×K | 1051.81 | Joback Method |
| cpg | 724.35 | J/mol×K | 1091.34 | Joback Method |

# Sources

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|---|---|
| **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=R537494&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **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 |