# Zearalenone bis(trifluoroacetate)

**Other names:** 17924-92-4, F3Ac
**Inchi:** InChI=1S/C22H20F6O7/c1-12-6-5-9-14(29)8-4-2-3-7-13-10-15(34-19(31)21(23,24)25)11
**InchiKey:** HPXZUGAUANXHJR-XVNBXDOJSA-N
**Formula:** C22H20F6O7
**SMILES:** CC1CCCC(=O)CCCC=Cc2cc(OC(=O)C(F)(F)F)cc(OC(=O)C(F)(F)F)c2C(=O)O1
**Mol. weight [g/mol]:** 510.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1762.63 | kJ/mol | Joback Method |
| hf | -2311.31 | kJ/mol | Joback Method |
| hfus | 42.29 | kJ/mol | Joback Method |
| hvap | 94.40 | kJ/mol | Joback Method |
| log10ws | -7.13 | | Crippen Method |
| logp | 5.104 | | Crippen Method |
| mcvol | 316.430 | ml/mol | McGowan Method |
| pc | 1339.80 | kPa | Joback Method |
| rinpol | 2409.00 | | NIST Webbook |
| rinpol | 2409.00 | | NIST Webbook |
| tb | 1093.04 | K | Joback Method |
| tc | 1342.30 | K | Joback Method |
| tf | 704.41 | K | Joback Method |
| vc | 1.200 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1084.52 | J/mol×K | 1093.04 | Joback Method |
| cpg | 1085.97 | J/mol×K | 1134.58 | Joback Method |
| cpg | 1084.03 | J/mol×K | 1176.13 | Joback Method |
| cpg | 1078.64 | J/mol×K | 1217.67 | Joback Method |
| cpg | 1069.74 | J/mol×K | 1259.21 | Joback Method |
| cpg | 1057.25 | J/mol×K | 1300.75 | Joback Method |
| cpg | 1041.12 | J/mol×K | 1342.30 | 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=U375714&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 |