

# (E)-2-Pentenal, PFBO # 1

**Inchi:** InChI=1S/C12H10F5NO/c1-2-3-4-5-18-19-6-7-8(13)10(15)12(17)11(16)9(7)14/h3-5H,2,6  
**InchiKey:** WYODGQGHSDKODJ-GWZFUMBFA-N  
**Formula:** C12H10F5NO  
**SMILES:** CCC=CC=NOc1c(F)c(F)c(F)c(F)c1F  
**Mol. weight [g/mol]:** 279.21

## Physical Properties

| Property code | Value    | Unit   | Source         |
|---------------|----------|--------|----------------|
| hf            | -1025.16 | kJ/mol | Joback Method  |
| hvap          | 49.49    | kJ/mol | Joback Method  |
| log10ws       | -5.20    |        | Crippen Method |
| logp          | 3.851    |        | Crippen Method |
| mcvol         | 172.280  | ml/mol | McGowan Method |
| pc            | 1723.16  | kPa    | Joback Method  |
| rinpol        | 1424.00  |        | NIST Webbook   |
| rinpol        | 1424.00  |        | NIST Webbook   |
| ripol         | 1808.00  |        | NIST Webbook   |
| ripol         | 1808.00  |        | NIST Webbook   |
| tb            | 625.15   | K      | Joback Method  |
| tc            | 808.30   | K      | Joback Method  |

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/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=R575545&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

|                  |   |
|------------------|---|
| <b>hf:</b>       | Enthalpy of formation at standard conditions    |
| <b>hvac:</b>     | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b>  | Log10 of Water solubility in mol/l              |
| <b>logp:</b>     | Octanol/Water partition coefficient             |
| <b>mcvol:</b>    | McGowan's characteristic volume                 |
| <b>pc:</b>       | Critical Pressure                               |
| <b>rinpolar:</b> | Non-polar retention indices                     |
| <b>ripolar:</b>  | Polar retention indices                         |
| <b>tb:</b>       | Normal Boiling Point Temperature                |
| <b>tc:</b>       | Critical Temperature                            |

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