# 1,2,3,4,7-Pentafluoro DBD

**Inchi:** InChI=1S/C12H3F5O2/c13-4-1-2-5-6(3-4)19-12-10(17)8(15)7(14)9(16)11(12)18-5/h1-3H
**InchiKey:** XDGUWUKXJWYIMN-UHFFFAOYSA-N
**Formula:** C12H3F5O2
**SMILES:** Fc1ccc2c(c1)Oc1c(F)c(F)c(F)c(F)c1O2
**Mol. weight [g/mol]:** 274.14

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -858.16 | kJ/mol | Joback Method |
| hf | -1043.49 | kJ/mol | Joback Method |
| hfus | 42.72 | kJ/mol | Joback Method |
| hvap | 56.48 | kJ/mol | Joback Method |
| log10ws | -4.64 | | Crippen Method |
| logp | 4.280 | | Crippen Method |
| mcvol | 142.150 | ml/mol | McGowan Method |
| pc | 2718.33 | kPa | Joback Method |
| rinpol | 1551.00 | | NIST Webbook |
| tb | 619.57 | K | Joback Method |
| tc | 823.63 | K | Joback Method |
| tf | 447.27 | K | Joback Method |
| vc | 0.590 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 352.10 | J/mol×K | 619.57 | Joback Method |
| cpg | 361.01 | J/mol×K | 653.58 | Joback Method |
| cpg | 369.34 | J/mol×K | 687.59 | Joback Method |
| cpg | 377.13 | J/mol×K | 721.60 | Joback Method |
| cpg | 384.42 | J/mol×K | 755.61 | Joback Method |
| cpg | 391.24 | J/mol×K | 789.62 | Joback Method |
| cpg | 397.65 | J/mol×K | 823.63 | 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=R223957&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 |