# Benzoic acid, 4-(pentafluoropropionylthio)-

**Inchi:** InChI=1S/C10H5F5O3S/c11-9(12,10(13,14)15)8(18)19-6-3-1-5(2-4-6)7(16)17/h1-4H,(H,1
**InchiKey:** HNRYQPURFRFAGK-UHFFFAOYSA-N
**Formula:** C10H5F5O3S
**SMILES:** O=C(O)c1ccc(SC(=O)C(F)(F)C(F)(F)F)cc1
**Mol. weight [g/mol]:** 300.20

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1193.81 | kJ/mol | Joback Method |
| hf | -1358.24 | kJ/mol | Joback Method |
| hfus | 27.30 | kJ/mol | Joback Method |
| hvap | 71.10 | kJ/mol | Joback Method |
| log10ws | -3.86 | | Crippen Method |
| logp | 3.201 | | Crippen Method |
| mcvol | 162.210 | ml/mol | McGowan Method |
| pc | 3038.96 | kPa | Joback Method |
| rinpol | 1512.00 | | NIST Webbook |
| rinpol | 1512.00 | | NIST Webbook |
| tb | 718.45 | K | Joback Method |
| tc | 920.35 | K | Joback Method |
| tf | 444.27 | K | Joback Method |
| vc | 0.640 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 429.72 | J/mol×K | 718.45 | Joback Method |
| cpg | 437.33 | J/mol×K | 752.10 | Joback Method |
| cpg | 444.22 | J/mol×K | 785.75 | Joback Method |
| cpg | 450.47 | J/mol×K | 819.40 | Joback Method |
| cpg | 456.13 | J/mol×K | 853.05 | Joback Method |
| cpg | 461.25 | J/mol×K | 886.70 | Joback Method |
| cpg | 465.88 | J/mol×K | 920.35 | 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=U375190&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 |

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