# Benzoic acid, 4-(heptafluorobutyrylthio)-

**Inchi:** InChI=1S/C11H5F7O3S/c12-9(13,10(14,15)11(16,17)18)8(21)22-6-3-1-5(2-4-6)7(19)20/h
**InchiKey:** KWCSMXGAMGRTQN-UHFFFAOYSA-N
**Formula:** C11H5F7O3S
**SMILES:** O=C(O)c1ccc(SC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc1
**Mol. weight [g/mol]:** 350.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1572.17 | kJ/mol | Joback Method |
| hf | -1779.85 | kJ/mol | Joback Method |
| hfus | 28.63 | kJ/mol | Joback Method |
| hvap | 70.40 | kJ/mol | Joback Method |
| log10ws | -4.60 | | Crippen Method |
| logp | 3.836 | | Crippen Method |
| mcvol | 179.840 | ml/mol | McGowan Method |
| pc | 2548.19 | kPa | Joback Method |
| rinpol | 1549.00 | | NIST Webbook |
| tb | 736.64 | K | Joback Method |
| tc | 931.53 | K | Joback Method |
| tf | 459.14 | K | Joback Method |
| vc | 0.722 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 498.19 | J/mol×K | 736.64 | Joback Method |
| cpg | 505.68 | J/mol×K | 769.12 | Joback Method |
| cpg | 512.47 | J/mol×K | 801.60 | Joback Method |
| cpg | 518.60 | J/mol×K | 834.08 | Joback Method |
| cpg | 524.16 | J/mol×K | 866.56 | Joback Method |
| cpg | 529.22 | J/mol×K | 899.04 | Joback Method |
| cpg | 533.84 | J/mol×K | 931.53 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U375186&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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 |

# 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 |