# 3-(Fluorosulfonyl)benzoic acid

**Other names:** Benzoic acid, 3-(fluorosulfonyl)-
m-(Fluorosulfonyl)benzoic acid
3-(fluorosulphonyl)benzoic acid
**Inchi:** InChI=1S/C7H5FO4S/c8-13(11,12)6-3-1-2-5(4-6)7(9)10/h1-4H,(H,9,10)
**InchiKey:** VWYMBWGOJRULOV-UHFFFAOYSA-N
**Formula:** C7H5FO4S
**SMILES:** O=C(O)c1cccc(S(=O)(=O)F)c1
**Mol. weight [g/mol]:** 204.18
**CAS:** 454-95-5

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -818.25 | kJ/mol | Joback Method |
| hf | -877.02 | kJ/mol | Joback Method |
| hfus | 27.68 | kJ/mol | Joback Method |
| hvap | 75.36 | kJ/mol | Joback Method |
| log10ws | -1.65 | | Crippen Method |
| logp | 1.043 | | Crippen Method |
| mcvol | 123.030 | ml/mol | McGowan Method |
| pc | 5836.07 | kPa | Joback Method |
| tb | 584.32 | K | Joback Method |
| tc | 778.52 | K | Joback Method |
| tf | 357.49 | K | Joback Method |
| vc | 0.488 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 275.17 | J/mol×K | 584.32 | Joback Method |
| cpg | 283.53 | J/mol×K | 616.69 | Joback Method |
| cpg | 291.35 | J/mol×K | 649.05 | Joback Method |
| cpg | 298.65 | J/mol×K | 681.42 | Joback Method |
| cpg | 305.42 | J/mol×K | 713.79 | Joback Method |
| cpg | 311.67 | J/mol×K | 746.15 | Joback Method |

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|---|---|---|---|---|
| cpg | 317.39 | J/mol×K | 778.52 | Joback Method |

# Sources

| | |
|---|---|
| **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=C454955&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |