# Benzoic acid, 2-(ethylthio)-, methyl ester

**Inchi:** InChI=1S/C10H12O2S/c1-3-13-9-7-5-4-6-8(9)10(11)12-2/h4-7H,3H2,1-2H3
**InchiKey:** OKRRVEHPTPIQOI-UHFFFAOYSA-N
**Formula:** C10H12O2S
**SMILES:** CCSc1ccccc1C(=O)OC
**Mol. weight [g/mol]:** 196.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -64.70 | kJ/mol | Joback Method |
| hf | -227.60 | kJ/mol | Joback Method |
| hfus | 22.23 | kJ/mol | Joback Method |
| hvap | 56.77 | kJ/mol | Joback Method |
| log10ws | -2.88 | | Crippen Method |
| logp | 2.585 | | Crippen Method |
| mcvol | 151.790 | ml/mol | McGowan Method |
| pc | 3089.85 | kPa | Joback Method |
| rinpol | 1581.00 | | NIST Webbook |
| tb | 604.93 | K | Joback Method |
| tc | 837.42 | K | Joback Method |
| tf | 347.96 | K | Joback Method |
| vc | 0.566 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 350.05 | J/mol×K | 604.93 | Joback Method |
| cpg | 363.45 | J/mol×K | 643.68 | Joback Method |
| cpg | 376.01 | J/mol×K | 682.43 | Joback Method |
| cpg | 387.72 | J/mol×K | 721.18 | Joback Method |
| cpg | 398.60 | J/mol×K | 759.92 | Joback Method |
| cpg | 408.65 | J/mol×K | 798.67 | Joback Method |
| cpg | 417.88 | J/mol×K | 837.42 | 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=U374956&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 |