# 4-(Methylthio)benzoic acid, 2,3,4,5-tetrafluorobenzyl ester

**Inchi:** InChI=1S/C15H10F4O2S/c1-22-10-4-2-8(3-5-10)15(20)21-7-9-6-11(16)13(18)14(19)12(9

**InchiKey:** NVCDWJONIKTYBW-UHFFFAOYSA-N

**Formula:** C15H10F4O2S

**SMILES:** CSc1ccc(C(=O)OCc2cc(F)c(F)c(F)c2F)cc1

**Mol. weight [g/mol]:** 330.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -727.95 | kJ/mol | Joback Method |
| hf | -924.59 | kJ/mol | Joback Method |
| hfus | 39.98 | kJ/mol | Joback Method |
| hvap | 69.55 | kJ/mol | Joback Method |
| log10ws | -5.89 | | Crippen Method |
| logp | 4.322 | | Crippen Method |
| mcvol | 205.560 | ml/mol | McGowan Method |
| pc | 2088.84 | kPa | Joback Method |
| rinpol | 2190.00 | | NIST Webbook |
| rinpol | 2190.00 | | NIST Webbook |
| tb | 763.01 | K | Joback Method |
| tc | 980.89 | K | Joback Method |
| tf | 483.17 | K | Joback Method |
| vc | 0.809 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 544.05 | J/mol×K | 763.01 | Joback Method |
| cpg | 555.69 | J/mol×K | 799.32 | Joback Method |
| cpg | 566.40 | J/mol×K | 835.64 | Joback Method |
| cpg | 576.18 | J/mol×K | 871.95 | Joback Method |
| cpg | 585.03 | J/mol×K | 908.26 | Joback Method |
| cpg | 592.97 | J/mol×K | 944.57 | Joback Method |
| cpg | 600.00 | J/mol×K | 980.89 | 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=U375061&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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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