# 2-(Methylthio)benzoic acid, 2-(trifluoromethyl)benzyl ester

**Inchi:** InChI=1S/C16H13F3O2S/c1-22-14-9-5-3-7-12(14)15(20)21-10-11-6-2-4-8-13(11)16(17,1

**InchiKey:** YYCQICSBJFLGGR-UHFFFAOYSA-N

**Formula:** C16H13F3O2S

**SMILES:** CSc1ccccc1C(=O)OCc1ccccc1C(F)(F)F

**Mol. weight [g/mol]:** 326.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -492.99 | kJ/mol | Joback Method |
| hf | -723.46 | kJ/mol | Joback Method |
| hfus | 33.24 | kJ/mol | Joback Method |
| hvap | 69.31 | kJ/mol | Joback Method |
| log10ws | -5.67 | | Crippen Method |
| logp | 4.784 | | Crippen Method |
| mcvol | 217.880 | ml/mol | McGowan Method |
| pc | 2113.89 | kPa | Joback Method |
| rinpol | 2179.00 | | NIST Webbook |
| rinpol | 2179.00 | | NIST Webbook |
| tb | 768.45 | K | Joback Method |
| tc | 1000.06 | K | Joback Method |
| tf | 458.71 | K | Joback Method |
| vc | 0.837 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 595.99 | J/mol×K | 768.45 | Joback Method |
| cpg | 609.14 | J/mol×K | 807.05 | Joback Method |
| cpg | 621.12 | J/mol×K | 845.65 | Joback Method |
| cpg | 631.98 | J/mol×K | 884.25 | Joback Method |
| cpg | 641.78 | J/mol×K | 922.85 | Joback Method |
| cpg | 650.58 | J/mol×K | 961.46 | Joback Method |
| cpg | 658.45 | J/mol×K | 1000.06 | 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=U375055&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |