

# Benzoic acid, 2-(methylthio)-, isopropyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C11H14O2S/c1-8(2)13-11(12)9-6-4-5-7-10(9)14-3/h4-8H,1-3H3

DWRKZLZVARMJKR-UHFFFAOYSA-N

C11H14O2S

CSc1ccccc1C(=O)OC(C)C

210.29

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -58.72  | kJ/mol  | Joback Method  |
| hf            | -253.52 | kJ/mol  | Joback Method  |
| hfus          | 21.29   | kJ/mol  | Joback Method  |
| hvap          | 58.60   | kJ/mol  | Joback Method  |
| log10ws       | -3.41   |         | Crippen Method |
| logp          | 2.974   |         | Crippen Method |
| mcvol         | 165.880 | ml/mol  | McGowan Method |
| pc            | 2808.38 | kPa     | Joback Method  |
| rinpol        | 1642.00 |         | NIST Webbook   |
| tb            | 627.37  | K       | Joback Method  |
| tc            | 860.16  | K       | Joback Method  |
| tf            | 344.23  | K       | Joback Method  |
| vc            | 0.616   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 398.78 | J/mol×K | 627.37          | Joback Method |
| cpg           | 413.29 | J/mol×K | 666.17          | Joback Method |
| cpg           | 426.85 | J/mol×K | 704.97          | Joback Method |
| cpg           | 439.46 | J/mol×K | 743.76          | Joback Method |
| cpg           | 451.15 | J/mol×K | 782.56          | Joback Method |
| cpg           | 461.92 | J/mol×K | 821.36          | Joback Method |
| cpg           | 471.77 | J/mol×K | 860.16          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U375375&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375375&amp;Units=SI</a> |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvac:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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