

# 2-Isobutyl-thiolane

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C8H16S/c1-7(2)6-8-4-3-5-9-8/h7-8H,3-6H2,1-2H3 |
| <b>InchiKey:</b>            | VNAMKUWAEAH CJL-UHFFFAOYSA-N                           |
| <b>Formula:</b>             | C8H16S   |
| <b>SMILES:</b>              | CC(C)CC1CCCS1  |
| <b>Mol. weight [g/mol]:</b> | 144.28   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 90.45   | kJ/mol               | Joback Method  |
| hf            | -107.99 | kJ/mol               | Joback Method  |
| hfus          | 10.54   | kJ/mol               | Joback Method  |
| hvap          | 39.08   | kJ/mol               | Joback Method  |
| log10ws       | -2.82   |                      | Crippen Method |
| logp          | 2.928   |                      | Crippen Method |
| mcvol         | 129.070 | ml/mol               | McGowan Method |
| pc            | 3072.75 | kPa                  | Joback Method  |
| rinpol        | 1080.00 |                      | NIST Webbook   |
| rinpol        | 1080.00 |                      | NIST Webbook   |
| tb            | 445.11  | K                    | Joback Method  |
| tc            | 658.20  | K                    | Joback Method  |
| tf            | 259.27  | K                    | Joback Method  |
| vc            | 0.465   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 263.46 | J/mol×K | 445.11          | Joback Method |
| cpg           | 280.56 | J/mol×K | 480.62          | Joback Method |
| cpg           | 296.73 | J/mol×K | 516.14          | Joback Method |
| cpg           | 312.00 | J/mol×K | 551.65          | Joback Method |
| cpg           | 326.40 | J/mol×K | 587.17          | Joback Method |
| cpg           | 339.97 | J/mol×K | 622.68          | Joback Method |
| cpg           | 352.75 | J/mol×K | 658.20          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=R405768&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R405768&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>hvap:</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>rinpola:</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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