

# 2-[But-3-enylthio]ethanal

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C6H10OS/c1-2-3-5-8-6-4-7/h2,4H,1,3,5-6H2 |
| <b>InchiKey:</b>            | VONVZGYHDWKQGY-UHFFFAOYSA-N                       |
| <b>Formula:</b>             | C6H10OS   |
| <b>SMILES:</b>              | C=CCCSCC=O  |
| <b>Mol. weight [g/mol]:</b> | 130.21  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 21.08   | kJ/mol               | Joback Method  |
| hf            | -85.45  | kJ/mol               | Joback Method  |
| hfus          | 16.43   | kJ/mol               | Joback Method  |
| hvap          | 41.82   | kJ/mol               | Joback Method  |
| log10ws       | -1.35   |                      | Crippen Method |
| logp          | 1.495   |                      | Crippen Method |
| mcvol         | 109.020 | ml/mol               | McGowan Method |
| pc            | 3624.61 | kPa                  | Joback Method  |
| ripol         | 1618.00 |                      | NIST Webbook   |
| ripol         | 1618.00 |                      | NIST Webbook   |
| tb            | 450.80  | K                    | Joback Method  |
| tc            | 650.46  | K                    | Joback Method  |
| tf            | 232.02  | K                    | Joback Method  |
| vc            | 0.423   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 208.90 | J/mol×K | 450.80          | Joback Method |
| cpg           | 218.68 | J/mol×K | 484.08          | Joback Method |
| cpg           | 228.00 | J/mol×K | 517.35          | Joback Method |
| cpg           | 236.87 | J/mol×K | 550.63          | Joback Method |
| cpg           | 245.30 | J/mol×K | 583.91          | Joback Method |
| cpg           | 253.29 | J/mol×K | 617.19          | Joback Method |
| cpg           | 260.87 | J/mol×K | 650.46          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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=R402096&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R402096&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>ripol:</b>   | 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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