

# Propargyl ethyl sulfide

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 3-(Ethylsulfanyl)-1-propyne<br>4-Thia-1-hexyne<br>Ethyl propargyl sulfide |
| <b>Inchi:</b>               | InChI=1S/C5H8S/c1-3-5-6-4-2/h1H,4-5H2,2H3                                 |
| <b>InchiKey:</b>            | HGRTUSIZMXOMCD-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C5H8S   |
| <b>SMILES:</b>              | C#CCSCC   |
| <b>Mol. weight [g/mol]:</b> | 100.18  |
| <b>CAS:</b>                 | 7310-92-1   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 247.41  | kJ/mol  | Joback Method  |
| hf            | 187.24  | kJ/mol  | Joback Method  |
| hfus          | 15.81   | kJ/mol  | Joback Method  |
| hvap          | 33.40   | kJ/mol  | Joback Method  |
| log10ws       | -1.59   |         | Crippen Method |
| logp          | 1.373   |         | Crippen Method |
| mcvol         | 89.060  | ml/mol  | McGowan Method |
| pc            | 4255.16 | kPa     | Joback Method  |
| rinpol        | 782.00  |         | NIST Webbook   |
| tb            | 372.70  | K       | Joback Method  |
| tc            | 577.46  | K       | Joback Method  |
| tf            | 227.48  | K       | Joback Method  |
| vc            | 0.332   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 146.79 | J/molxK | 372.70          | Joback Method |
| cpg           | 154.92 | J/molxK | 406.83          | Joback Method |
| cpg           | 162.68 | J/molxK | 440.95          | Joback Method |
| cpg           | 170.09 | J/molxK | 475.08          | Joback Method |
| cpg           | 177.15 | J/molxK | 509.21          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 183.88 | J/mol×K | 543.34 | Joback Method |
| cpg | 190.28 | J/mol×K | 577.46 | 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=C7310921&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7310921&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>rinpolar:</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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