

# 3-Mercaptopropyl-1-acetate

Inchi:

InChI=1S/C5H10O2S/c1-5(6)7-3-2-4-8/h8H,2-4H2,1H3

InchiKey:

FVSBSLZVZIYRRO-UHFFFAOYSA-N

Formula:

C5H10O2S

SMILES:

CC(=O)OCCCS

Mol. weight [g/mol]:

134.20

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -213.31 | kJ/mol  | Joback Method  |
| hf            | -352.85 | kJ/mol  | Joback Method  |
| hfus          | 15.53   | kJ/mol  | Joback Method  |
| hvap          | 42.62   | kJ/mol  | Joback Method  |
| log10ws       | -0.85   |         | Crippen Method |
| logp          | 0.869   |         | Crippen Method |
| mcvol         | 105.100 | ml/mol  | McGowan Method |
| pc            | 3965.51 | kPa     | Joback Method  |
| rinpol        | 992.00  |         | NIST Webbook   |
| rinpol        | 992.00  |         | NIST Webbook   |
| tb            | 452.95  | K       | Joback Method  |
| tc            | 654.90  | K       | Joback Method  |
| tf            | 254.73  | K       | Joback Method  |
| vc            | 0.394   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 204.20 | J/mol×K | 452.95          | Joback Method |
| cpg           | 213.49 | J/mol×K | 486.61          | Joback Method |
| cpg           | 222.42 | J/mol×K | 520.27          | Joback Method |
| cpg           | 231.01 | J/mol×K | 553.93          | Joback Method |
| cpg           | 239.23 | J/mol×K | 587.58          | Joback Method |
| cpg           | 247.10 | J/mol×K | 621.24          | Joback Method |
| cpg           | 254.60 | J/mol×K | 654.90          | 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=R603348&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R603348&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>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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