# 3-mercaptooctyl-acetate

**Inchi:** InChI=1S/C10H20O2S/c1-3-4-5-6-10(13)7-8-12-9(2)11/h10,13H,3-8H2,1-2H3
**InchiKey:** WMRTWAVKXSNZCF-UHFFFAOYSA-N
**Formula:** C10H20O2S
**SMILES:** CCCCCC(S)CCOC(C)=O
**Mol. weight [g/mol]:** 204.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -173.65 | kJ/mol | Joback Method |
| hf | -461.33 | kJ/mol | Joback Method |
| hfus | 24.96 | kJ/mol | Joback Method |
| hvap | 53.36 | kJ/mol | Joback Method |
| log10ws | -3.05 | | Crippen Method |
| logp | 2.818 | | Crippen Method |
| mcvol | 175.550 | ml/mol | McGowan Method |
| pc | 2356.49 | kPa | Joback Method |
| rinpol | 1425.00 | | NIST Webbook |
| rinpol | 1425.00 | | NIST Webbook |
| ripol | 1930.00 | | NIST Webbook |
| ripol | 1930.00 | | NIST Webbook |
| tb | 566.91 | K | Joback Method |
| tc | 760.21 | K | Joback Method |
| tf | 296.08 | K | Joback Method |
| vc | 0.667 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 422.94 | J/mol×K | 566.91 | Joback Method |
| cpg | 437.78 | J/mol×K | 599.13 | Joback Method |
| cpg | 451.94 | J/mol×K | 631.34 | Joback Method |
| cpg | 465.43 | J/mol×K | 663.56 | Joback Method |
| cpg | 478.26 | J/mol×K | 695.77 | Joback Method |
| cpg | 490.44 | J/mol×K | 727.99 | Joback Method |

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|---|---|---|---|---|
| cpg | 501.97 | J/mol×K | 760.21 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R291831&Units=SI |

# Legend

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