# 3-Methyl-3-sulfanylbutyl Hexadecanoate

**Inchi:** InChI=1S/C21H42O2S/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20(22)23-19-18-21(2,3)2
**InchiKey:** KLURJANGYPXWHJ-UHFFFAOYSA-N
**Formula:** C21H42O2S
**SMILES:** CCCCCCCCCCCCCCCC(=O)OCCC(C)(C)S
**Mol. weight [g/mol]:** 358.62

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -75.75 | kJ/mol | Joback Method |
| hf | -691.84 | kJ/mol | Joback Method |
| hfus | 49.56 | kJ/mol | Joback Method |
| hvap | 76.94 | kJ/mol | Joback Method |
| log10ws | -7.66 | | Crippen Method |
| logp | 7.109 | | Crippen Method |
| mcvol | 330.540 | ml/mol | McGowan Method |
| pc | 1037.23 | kPa | Joback Method |
| rinpol | 2492.00 | | NIST Webbook |
| tb | 815.80 | K | Joback Method |
| tc | 1005.36 | K | Joback Method |
| tf | 437.47 | K | Joback Method |
| vc | 1.278 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1037.87 | J/mol×K | 815.80 | Joback Method |
| cpg | 1057.35 | J/mol×K | 847.39 | Joback Method |
| cpg | 1075.76 | J/mol×K | 878.99 | Joback Method |
| cpg | 1093.12 | J/mol×K | 910.58 | Joback Method |
| cpg | 1109.51 | J/mol×K | 942.18 | Joback Method |
| cpg | 1124.95 | J/mol×K | 973.77 | Joback Method |
| cpg | 1139.51 | J/mol×K | 1005.36 | Joback Method |

# Sources

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|---|---|
| **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=R519585&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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|---|---|
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |