# 3-Methyl-3-sulfanylbutyl Tetradecanoate

**Inchi:** InChI=1S/C19H38O2S/c1-4-5-6-7-8-9-10-11-12-13-14-15-18(20)21-17-16-19(2,3)22/h22
**InchiKey:** FXRSTAIWMGQKTN-UHFFFAOYSA-N
**Formula:** C19H38O2S
**SMILES:** CCCCCCCCCCCCCC(=O)OCCC(C)(C)S
**Mol. weight [g/mol]:** 330.57

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -92.59 | kJ/mol | Joback Method |
| hf | -650.56 | kJ/mol | Joback Method |
| hfus | 44.38 | kJ/mol | Joback Method |
| hvap | 72.48 | kJ/mol | Joback Method |
| log10ws | -6.82 | | Crippen Method |
| logp | 6.329 | | Crippen Method |
| mcvol | 302.360 | ml/mol | McGowan Method |
| pc | 1178.47 | kPa | Joback Method |
| rinpol | 2287.00 | | NIST Webbook |
| rinpol | 2287.00 | | NIST Webbook |
| ripol | 2770.00 | | NIST Webbook |
| ripol | 2770.00 | | NIST Webbook |
| tb | 770.04 | K | Joback Method |
| tc | 957.18 | K | Joback Method |
| tf | 414.93 | K | Joback Method |
| vc | 1.167 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 916.80 | J/mol×K | 770.04 | Joback Method |
| cpg | 935.70 | J/mol×K | 801.23 | Joback Method |
| cpg | 953.58 | J/mol×K | 832.42 | Joback Method |
| cpg | 970.48 | J/mol×K | 863.61 | Joback Method |
| cpg | 986.44 | J/mol×K | 894.80 | Joback Method |
| cpg | 1001.51 | J/mol×K | 925.99 | Joback Method |

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|---|---|---|---|---|
| cpg | 1015.72 | J/mol×K | 957.18 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R519629&Units=SI |
| **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 |

# 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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |