# 3-Sulfanylhexyl Hexadodecanoate

**Inchi:** InChI=1S/C22H44O2S/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-18-22(23)24-20-19-21(25)1
**InchiKey:** STJAWXNXWLRHTH-UHFFFAOYSA-N
**Formula:** C22H44O2S
**SMILES:** CCCCCCCCCCCCCCCC(=O)OCCC(S)CCC
**Mol. weight [g/mol]:** 372.65

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -72.61 | kJ/mol | Joback Method |
| hf | -709.01 | kJ/mol | Joback Method |
| hfus | 56.04 | kJ/mol | Joback Method |
| hvap | 80.07 | kJ/mol | Joback Method |
| log10ws | -8.08 | | Crippen Method |
| logp | 7.500 | | Crippen Method |
| mcvol | 344.630 | ml/mol | McGowan Method |
| pc | 969.28 | kPa | Joback Method |
| rinpol | 2615.00 | | NIST Webbook |
| tb | 841.47 | K | Joback Method |
| tc | 1032.20 | K | Joback Method |
| tf | 431.32 | K | Joback Method |
| vc | 1.339 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1099.51 | J/mol×K | 841.47 | Joback Method |
| cpg | 1119.42 | J/mol×K | 873.26 | Joback Method |
| cpg | 1138.17 | J/mol×K | 905.05 | Joback Method |
| cpg | 1155.82 | J/mol×K | 936.83 | Joback Method |
| cpg | 1172.40 | J/mol×K | 968.62 | Joback Method |
| cpg | 1187.95 | J/mol×K | 1000.41 | Joback Method |
| cpg | 1202.50 | J/mol×K | 1032.20 | Joback Method |

# Sources

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|---|---|
| **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=R519669&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |