# N-3-(Methylthio)propyl O-propyl thiocarbamate

**Inchi:** InChI=1S/C8H17NOS2/c1-3-6-10-8(11)9-5-4-7-12-2/h3-7H2,1-2H3,(H,9,11)
**InchiKey:** YAJCCTPNVXDAOW-UHFFFAOYSA-N
**Formula:** C8H17NOS2
**SMILES:** CCCOC(=S)NCCCSC
**Mol. weight [g/mol]:** 207.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 151.05 | kJ/mol | Joback Method |
| hf | -98.83 | kJ/mol | Joback Method |
| hfus | 31.50 | kJ/mol | Joback Method |
| hvap | 55.79 | kJ/mol | Joback Method |
| log10ws | -2.68 | | Crippen Method |
| logp | 2.041 | | Crippen Method |
| mcvol | 167.830 | ml/mol | McGowan Method |
| pc | 2826.33 | kPa | Joback Method |
| rinpol | 1730.00 | | NIST Webbook |
| rinpol | 1730.00 | | NIST Webbook |
| ripol | 2770.00 | | NIST Webbook |
| tb | 593.85 | K | Joback Method |
| tc | 803.02 | K | Joback Method |
| tf | 323.48 | K | Joback Method |
| vc | 0.626 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 395.07 | J/mol×K | 593.85 | Joback Method |
| cpg | 408.16 | J/mol×K | 628.71 | Joback Method |
| cpg | 420.54 | J/mol×K | 663.57 | Joback Method |
| cpg | 432.22 | J/mol×K | 698.43 | Joback Method |
| cpg | 443.25 | J/mol×K | 733.30 | Joback Method |
| cpg | 453.64 | J/mol×K | 768.16 | Joback Method |
| cpg | 463.43 | J/mol×K | 803.02 | Joback Method |

# Sources

| | |
|---|---|
| **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=R440018&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |