# 5-heptyl-dihydrofuran-2(3H)-thione

**Inchi:** InChI=1S/C11H18OS/c1-2-3-4-5-6-7-10-8-9-11(13)12-10/h8H,2-7,9H2,1H3
**InchiKey:** NLGVCAHTJNYDCN-UHFFFAOYSA-N
**Formula:** C11H18OS
**SMILES:** CCCCCCCC1=CCC(=S)O1
**Mol. weight [g/mol]:** 198.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 111.06 | kJ/mol | Joback Method |
| hf | -160.14 | kJ/mol | Joback Method |
| hfus | 31.96 | kJ/mol | Joback Method |
| hvap | 53.59 | kJ/mol | Joback Method |
| log10ws | -4.61 | | Crippen Method |
| logp | 3.978 | | Crippen Method |
| mcvol | 168.610 | ml/mol | McGowan Method |
| pc | 2537.93 | kPa | Joback Method |
| ripol | 2490.00 | | NIST Webbook |
| tb | 574.76 | K | Joback Method |
| tc | 782.28 | K | Joback Method |
| tf | 332.39 | K | Joback Method |
| vc | 0.638 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 405.42 | J/mol×K | 574.76 | Joback Method |
| cpg | 420.26 | J/mol×K | 609.35 | Joback Method |
| cpg | 434.23 | J/mol×K | 643.93 | Joback Method |
| cpg | 447.38 | J/mol×K | 678.52 | Joback Method |
| cpg | 459.78 | J/mol×K | 713.11 | Joback Method |
| cpg | 471.47 | J/mol×K | 747.69 | Joback Method |
| cpg | 482.50 | J/mol×K | 782.28 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R422496&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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |