# 2-(1,3-octadienyl)-4,5-dimethyl-3-thiazoline, trans

**Inchi:** InChI=1S/C13H21NS/c1-4-5-6-7-8-9-10-13-14-11(2)12(3)15-13/h7-10,12-13H,4-6H2,1-3

**InchiKey:** DLSYFVPFFOKHTD-ICQRHVMVSA-N

**Formula:** C13H21NS

**SMILES:** CCCCC=CC=CC1N=C(C)C(C)S1

**Mol. weight [g/mol]:** 223.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 424.83 | kJ/mol | Joback Method |
| hf | 125.47 | kJ/mol | Joback Method |
| hfus | 34.46 | kJ/mol | Joback Method |
| hvap | 57.37 | kJ/mol | Joback Method |
| log10ws | -4.63 | | Crippen Method |
| logp | 4.211 | | Crippen Method |
| mcvol | 196.600 | ml/mol | McGowan Method |
| pc | 2068.00 | kPa | Joback Method |
| rinpol | 1792.00 | | NIST Webbook |
| tb | 621.44 | K | Joback Method |
| tc | 843.40 | K | Joback Method |
| tf | 401.04 | K | Joback Method |
| vc | 0.745 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 515.67 | J/mol×K | 621.44 | Joback Method |
| cpg | 535.16 | J/mol×K | 658.43 | Joback Method |
| cpg | 553.44 | J/mol×K | 695.43 | Joback Method |
| cpg | 570.59 | J/mol×K | 732.42 | Joback Method |
| cpg | 586.64 | J/mol×K | 769.41 | Joback Method |
| cpg | 601.65 | J/mol×K | 806.40 | Joback Method |
| cpg | 615.68 | J/mol×K | 843.40 | 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=R497495&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |